

DEPARTMENT OF MATHEMATICS & STATISTICS
COLLEGE OF SCIENCES
OLD DOMINION UNIVERSITY
NORFOLK, VIRGINIA 23529

**WAVELET DENOISING OF RADAR SIGNALS, REVERSE
ENGINEERING FOR AIRCRAFT DESIGN, AND
OPTIMIZATION METHOD**

By

Wu Li, Principal Investigator

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Final Report

For the period November 1, 1994 through October 31, 1995

Prepared for
AFOSR/NM
110 Duncan Avenue, Suite B115
Bolling AFB, DC 20332-0001

Under
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Dr. Jon A. Sjogren, Program Manager

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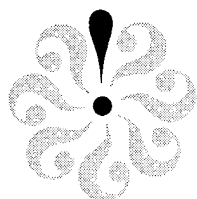
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Final Report of Project F49620-95-1-0045 on Wavelet Denoising, Reverse Engineering, and Optimization

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January 17, 1996

Abstract

During the past year, we worked on two engineering application problems: data smoothing/denoising by wavelets and reverse engineering for aircraft design, as well as other optimization problems (such as robust regressions, Huber M-estimators, merit functions for constrained minimization problems, stability analysis of feasible systems, and constrained best approximations in Euclidean spaces). While the engineering applications are obviously beneficial to the advancement of science and technology for Air Force, the basic research is also fundamental for potential applications relevant to Air Force. In this final report, we will give an overview of what we have accomplished during the last one year when our research was supported by Air Force Office of Scientific Research.

The report has five parts: (i) automatic threshold selection for wavelet denoising; (ii) reverse engineering for aircraft design; (iii) robust regression and Huber M-estimator; (iv) global error bounds for quadratic inequalities; (v) merit functions for complementarity problems.

1 Automatic Threshold Selection for Wavelet Denoising

Recently, one major trend in wavelet research is an *optimal* representation of a signal by a library (or dictionary) of basis functions, led by Mallat, Coifman, and Donoho [1, 2, 3, 4, 8]. The mathematical objective is to find a representation of a signal by a linear combination of as few functions in the library as possible within certain error tolerance. The motivation for such an optimal representation of a signal is to achieve data compression, since one only has to store the coefficients an approximate representation of the actual signal.

However, such an optimal representation is useful not only for data compression, but also for denoising of signals and feature extraction of speech signals, as pointed out by Buckheit and Donoho [1]. Our preliminary research [5] as well as Buckheit and Donoho's indicates that wavelet packet representation may provide better feature extraction than other classical classification method, such as linear discriminant analysis. Here we first give a brief review on denoising and feature extraction by wavelets. Then we report our progress made on Donoho and Johnstone's wavelet denoising method for recovering antenna radiation pattern from noisy measurements.

1.1 Review on Denoising and Feature Extraction

The wavelet packet transform is generated by a pair of quadratic mirror filters which decompose the signal into a series of subbands ("frequency slots") by repeated convolution and decimation. The wavelet packet coefficients generated by such a transform represent the energy levels of the signal at different time locations and various frequency bands. With appropriate choice of subbands and filters, it is possible to "capture" the signal with very few significantly large coefficients.

Let $\{g(n)\}_{n=1}^L$ (high-frequency filter) and $\{h(n)\}_{n=1}^L$ ($g(n) = (-1)^n h(1-n)$) (low-frequency filter) be a pair of finite impulse response (FIR) quadrature filters (QF) that correspond the coefficients in the equations that define scaling and mother wavelet functions:

$$\begin{aligned}\varphi(t) &= \sum_n h(n)\varphi(2t - n), \\ \psi(t) &= \sum_n g(n)\varphi(2t - n),\end{aligned}$$

where φ is the scaling function and ψ is the mother wavelet.

Given a sequence $\{x(j)\}_{j=1}^N$ of N samples of a signal, one can separate the frequency domain of the signal into two subbands of the same width by using the following transformation:

$$\begin{aligned} y_1(k) &= \sum_n h(n)x(2k-n), \\ y_0(k) &= \sum_n g(n)x(2k-n), \end{aligned} \quad (1)$$

where y_0 and y_1 contain the information of the signal in the high and low frequency subbands, respectively. The coefficients $y_0(k)$'s and $y_1(k)$'s are called wavelet packet coefficients at the first level. Repeating the same operation on a subband, we can get better frequency separation of the signal at the cost of lower resolution in time domain for the signal representation. This phenomena is dictated by the uncertainty principle in signal processing. For speech recognition problems, the design of subbands for the wavelet packet transform of signals is a very important issue, since a signal tends to have energy concentrated on certain frequency bands. If these subbands are used in the wavelet packet transform, then one might be able to use a few coefficients in these subbands to represent the signal. As a result, one can achieve data compression of the signal (a compressed representation of the signal by a few coefficients). This compressed representation can be used for either denoising or feature extraction. If one uses these coefficients to reconstruct a signal by the inverse wavelet packet transform (the transform (1) is invertible), then it will be a smoothed version of the original signal. This is the idea behind wavelet shrinkage for denoising. However, if one uses these coefficients as the input of a classification program, such as a neural network or a multisurface method of pattern separation [20], then these coefficients are called features of the signal in speech recognition [1, 5]. Therefore, the compressed representation of the signal provides a new approach for feature extraction in speech recognition.

For a special wavelet packet transform, we get a set of wavelet packet coefficients from the input signal $\{x(k)\}_{k=1}^{N=2^m}$:

$$\{w_{i,j} : i = 1, \dots, s, j = 1, \dots, 2^{r_i}\},$$

where $w_{i,j}$ represents the energy concentration at the i -th frequency subband and near the time location $\frac{j-1}{2^{r_i}}T$. The parameter T is the time duration of the signal: $T = \frac{N}{S}$, where S is the sampling rate of the signal.

For speech recognition problems, instead of finding a best basis for all signals [1], we used the averages of wavelet packet coefficients $w_{i,j}$'s as fea-

tures [5]. For isolated stops, the six consonants /b,p,d,t,g,k/ can be automatically classified with over 93% accuracy based on extracting 83 features out of a 75 ms signal interval beginning with the release of the burst. For stops extracted from continuous speech samples, we achieve an accuracy of 71% using 99 features out of an 83 ms signal interval. These relatively poor results are still comparable with a method using formant trajectories. However, they are not yet as good as results based on smoothed time/frequency features [5]. One possible reason is that each class of consonants has certain ridge signatures on the time/frequency plane and the features based on ridge signatures reflect more of the characteristics of speech signals.

As for signals received by antenna radiation pattern measurement equipment, we realized that the radar pattern nulls were mistaken as noisy spikes and were suppressed by wavelet shrinkage method for denoising. This confirms Coifman and Donoho's conclusion that pseudo-Gibbs phenomena happens in the neighborhood of discontinuities [3]. They attribute this to the lack of translation invariance of the wavelet basis. Their strategy to reduce the Gibbs phenomena is to average out the translation dependence by shifting the signal, denoising the shifted signal, and unshifting the smoothed signal. The method is called translation-invariant denoising [3]. Whether such a method can be used to preserve the radar pattern nulls remains to be seen.

1.2 Progress on Wavelet Denoising

Given $N(= 2^k)$ samples of a signal, from the statistical theory about the optimal minimax rate of convergence established by Donoho and Johnstone, we know that it is desirable to choose level-dependent thresholds based on the standard deviation of the noise signal. For example, Donoho and Johnstone proposed to use the following thresholds for thresholding of wavelet coefficients:

$$\sigma_i = c_i \sigma, \quad (2)$$

where c_i are some constants. The level-dependent thresholding can be considered as a black box that takes a set of wavelet coefficients $\{w_{i,j} : 1 \leq j \leq 2^{i-1}, 1 \leq i \leq k\}$ and output another set of wavelet coefficients:

$$\{\bar{w}_{i,j} : 1 \leq j \leq 2^{i-1}, 1 \leq i \leq k\},$$

where $\bar{w}_{i,j} = 0$ if $|w_{i,j}| \leq \sigma_i$ and $\bar{w}_{i,j} = w_{i,j} \left(1 - \frac{\sigma}{|w_{i,j}|}\right)$ otherwise. Then one can construct a unique signal $\bar{x}_1, \dots, \bar{x}_n$ corresponding to the modified

wavelet coefficients $\bar{w}_{i,j}$. By the results established by Donoho and Johnstone, we can consider \bar{x} as an optimal recovery of the uncontaminated signal in the minimax sense.

However, in a practical situation, the standard deviation of the noise signal is generally unknown. This causes a serious problem for engineers who would apply the wavelet denoising method in applications. In order to derive a practical method for automatic selection of the threshold, we need to consider the threshold selection from a different perspective. Suppose that we know the standard deviation σ of the noise signal ϵ . Then the thresholds for various levels defined in (2) yield an optimal recovery \bar{x} from x . Intuitively, we can assume that, with a high probability, \bar{x} is very close to the uncontaminated signal. That is, $x - \bar{x}$ should be very close to the noise signal ϵ . As a result, the standard deviation $\bar{\sigma}$ of $x - \bar{x}$ is approximately σ . Therefore, one statistical criterion for a good estimate σ of the standard deviation of the noise is that $\bar{\sigma} \approx \sigma$.

To implement such an idea, we use a control parameter $\delta(> 0)$ as the error tolerance of the threshold estimate. Then we try to find the largest σ such that $\left| \frac{\sigma - \bar{\sigma}}{\sigma} \right| \leq \delta$.

If one wants the optimal choice of σ , then one has to solve the nondifferentiable global minimization problem:

$$\min_{\sigma > 0} \left| \frac{\sigma - \bar{\sigma}}{\sigma} \right| =: g(\sigma).$$

Note that $\lim_{\sigma \rightarrow \infty} g(\sigma) = \lim_{\sigma \rightarrow 0} g(\sigma) = 1$. Therefore, the above minimization has a global solution.

We implemented the automatic threshold selection for wavelet shrinkage denoising. The application of this method to signals received by antenna radiation pattern measurement equipment at Airforce Rome Lab shows that the method can recover the noise-free signal quite accurately near the main-lobe and dominant sidelobes (cf. Figures 8 and 9). Such a denoising technique not only provides a smoothed signal, but also gives an empirical estimate of the standard deviation of the noisy signal.

A potential application of such a denoising technique is to filter out the noise in antenna radiation pattern measurement so that the true antenna gain pattern versus orientation angle can be discerned. Antennas that operate at 40 GHz and above are being developed that need to be tested against their design characteristics. This means that power amplifiers capable of operating at these frequencies are also required for far-field antenna pattern

measurement. These state-of-the-art amplifiers are either costly or nonexistent. Thus, getting the most signal-to-noise ratio is essential for reducing measurement costs.

1.3 Conclusions

As we pointed out before, the radar pattern nulls can be easily mistaken as noise by a nonparametric data smoothing/denoising method. For example, Donoho and Johnstone's wavelet shrinkage denoising method might destroy the null structure near the sidelobes (compare the smoothed signal and noiseless signal between -40 — -30 in Figure 9). One approach for maintaining the null structure is to set lower thresholds near the nulls for wavelet coefficients corresponding to high frequency subbands to preserve the null structure. We will continue to explore various denoising approaches for processing of signals received by antenna radiation pattern measurement equipment and our objective is to make a technology transition of the state-of-art wavelet denoising techniques to Airforce.

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2 Reverse Engineering for Aircraft Design

Reverse engineering is a relatively new term that emerged in the late 1980's. In general, reverse engineering is a process that begins with a physical form and ends with a computer representation of the form. With the recent developments of advanced laser digitizers and other computer-aided tools, reverse engineering has evolved from a research initiative to an industrial reality.

Reverse engineering has multiple applications, including the following:

- manufacturing a mechanical part from a new physical model or prototype,
- replicating an existing mechanical part that does not have a computer-recognizable design,
- analyzing or modifying a mechanical part that does not have a computer-recognizable design,
- verifying a mechanical part that has a computer-recognizable design [3].

Reverse engineering consists of four steps: data acquisition, data separation, curve or surface fitting, computer-aided manufacturing. Data acquisition is the collection of data points from the surface of a object. Normally, this is done by using a coordinate measuring machine (CMM) or a laser scanner. Because most objects are complicated (i.e., they are the composite of multiple geometric shapes), it is difficult to represent the object with one mathematical surface. Therefore, it is natural to separate the collected data into several components with simple geometric shapes. Then, one can fit a curve or surface equation to the data of each component. Together these equations provide a mathematical surface representation of the object. This representation or mathematical surface model can be programmed into computer-aided manufacturing (CAM) tools, which are used to manufacture a facimile of the original object.

From a mathematical point of view, the difficulty of the reverse engineering process is the construction of surface equations from a set of data points. There are software packages that were developed recently for the reverse engineering process, rather than for engineering design. Examples of these packages are "SURFACER" by Imageware, Inc., and "STRIM" by Matra Datavision. However, each application imposes different criteria for goodness-of-fit. For example, the objective of reverse engineering a car model is complete different from that of reverse engineering an aircraft model. The former has more emphasis on aesthetics and the latter has more emphasis on geometric shape and accuracy.

The main purpose of reverse engineering an aircraft surface is to use the original model as a starting point to design experimental aircraft. Historically, aircraft design has been divided into three phases: (1) conceptual design; (2) preliminary design; and (3) detailed design. A new methodology is to use a multi-disciplinary optimization (MDO) approach that combines surface geometry design, surface or volume grid generation, and aerodynamic optimization based on CFD analysis. With the MDO approach, the designer takes an existing surface design, generates the appropriate grids, and performs a CFD analysis of the design. The designer uses the analysis to identify aerodynamic features that are not optimal. The designer then modifies the design parameters associated with the aerodynamic features. This generates a new surface design. The designer repeats this process until he achieves the model with the desired aerodynamic features.

The MDO approach does have some serious difficulties. First, if the surface model has too many design parameters, the computational cost to optimize with respect to design parameters may be prohibitive. Second, design parameters within feasible ranges produce smooth surfaces (i.e., surfaces without ripples). When spline control points are used as design parameters, it is difficult to determine the relationship between the control points and the surface ripples.

To avoid these difficulties, a practical approach is to use a small set of engineering parameters to generate an aircraft model. This is the basic idea behind the Rapid Aircraft Parameter Input Design (RAPID) model, developed by Bloor, Wilson, and Smith [10]. With respect to the RAPID model, the reverse engineering problem is to determine the engineering design parameters from a set of aircraft surface data points. Then, one can optimize the aerodynamic features of the model by modifying the appropriate parameters.

In this section, based on Bloor and Wilson's PDE surface model, we use

a nonlinear least squares method to extract a set of engineering parameters from surface grids of an aircraft.

For more details, see the joint paper written by J. Huband, R. Smith, and the principle investigator [4].

2.1 Review on Reverse Engineering

For surface reconstruction in reverse engineering problems, one has to derive a parametric surface representation of a set of data points $\{(x_i, y_i, z_i)\}_{i=1}^n$ in space \mathbf{R}^3 :

$$x = x(u, v), \quad y = y(u, v), \quad z = z(u, v), \quad \text{for } 0 \leq u, v \leq 1. \quad (3)$$

The standard procedure for constructing a surface from $S \equiv \{(x_i, y_i, z_i)\}_{i=1}^n$ is a three-step process:

- selection of 4 sets B_1, B_2, B_3, B_4 of ordered boundary points from S ;
- fitting of a spline curve C_i of each boundary set B_i such that C_1, C_2, C_3, C_4 form a closed loop;
- construction of a surface based on 4 boundary curves C_1, C_2, C_3, C_4 and the data set S .

There are many papers on construction of a surface from the data set S if $z_i = f(x_i, y_i)$ and (x_i, y_i) are in a rectangular region or S is a set of grid points on a surface [1, 2, 3, 6, 7, 8]. However, for digitized surface of a mechanical part such as a wing of an aircraft, there is no structure pattern for S . At NASA Langley Research Center, the surface construction is done by using a state-of-art reverse engineering software called SURFACER [9] developed by Imageware Inc. The selection of boundary points has to be done manually through a point clicking interface. Even though the interface is very easy to use, the process is quite tedious and time-consuming. The fitting process used by SURFACER is a variation of thin spline fitting, which is very sensitive to the results of boundary curve fitting. For example, the knots for the final surface are completely predetermined by the knots of the boundary curves. As a consequence, a successful surface construction relies on the expertise of a designer/modeller who goes through many trials of boundary and surface fitting to get a visually satisfactory result. The major difficulty in such a surface construction process is how to determine

the corresponding parameter (u_i, v_i) of (x_i, y_i, z_i) for a given parametric form of surfaces (3). There is no mathematical research done so far on this topic.

For aircraft designs, a spline surface does not make much sense to engineers. Therefore, surface models based on engineering (or geometric) parameters (such as the wing section chord length, the wing section maximum thickness, the location of maximum camber, cf. Figures 3-7 by Robert Smith at NASA/Langley Research Center) are very important for modification of a given design. Smith, Bloor, Wilson, and Thomas [10] developed a RAPID prototyping model for airplane design at NASA Langley Research Center. However, in order to make the software applicable in practice, one has to convert the surface grids of a given airplane to a RAPID model. Then one can modify the RAPID model to derive a design with optimal aerodynamic characteristics. This often involves a multidisciplinary design optimization process.

2.2 Progress on Surface Reconstruction in Reverse Engineering

Our major contribution is to reverse the following PDE model for rapid prototyping of an aircraft:

$$\left(\frac{\partial^2}{\partial \eta^2} + \left(\frac{a}{2\pi} \right)^2 \frac{\partial^2}{\partial \xi^2} \right)^2 F(\xi, \eta) = 0, \quad \text{for } 0 \leq \eta, \xi \leq 1, \quad (4)$$

$$F(0, \eta) = F(1, \eta), \quad \text{for } 0 \leq \eta \leq 1, \quad (5)$$

$$F(\xi, 0) = B_0(\xi), \quad F(\xi, 1) = B_1(\xi), \quad \text{for } 0 \leq \xi \leq 1, \quad (6)$$

$$\frac{\partial F}{\partial \eta}(\xi, 0) = N_0(\xi), \quad \frac{\partial F}{\partial \eta}(\xi, 1) = N_1(\xi), \quad \text{for } 0 \leq \xi \leq 1, \quad (7)$$

where (5) forces the solution to be a periodic function of ξ with period $T = 1$, (6) is the Dirichlet boundary condition, and (7) is the Neumann boundary condition.

It is well-known that the fourth-order elliptic PDE (4) with the given boundary conditions has a unique solution. This provides a way of generating a surface patch with the given Dirichlet and Neumann boundary conditions, which is the mathematical foundation of Bloor and Wilson's idea for rapid prototyping of an aircraft and other rapid prototyping applications.

For example, in the design of the inboard wing section, one usually specifies the two airfoils at the two ends of the inboard wing section (which are the intersection of the inboard/outboard wing sections and the intersection of

the inboard wing/fuselage), as well as how smooth the inboard wing section blends with the fuselage and the outboard wing section. Note that the two airfoils are given as boundary functions $B_0(\xi)$ and $B_1(\xi)$, while the smoothness of blending is represented by boundary functions $N_0(\xi)$ and $N_1(\xi)$. Therefore, construction of the wing section is mathematically equivalent to construction of a smooth surface that satisfies the boundary conditions (6) and (7). For the inboard wing section, the boundary functions are given as follows:

$$B_0(\xi) = \begin{pmatrix} x = \bar{x}(\xi) + X_c \\ y = R_0 + H_1 \\ z = \bar{y}(\xi) + Z_c \end{pmatrix}, \quad B_1(\xi) = \begin{pmatrix} x = \frac{B_w}{C} \bar{x}(\xi) + X_w \\ y = \sqrt{r(\xi)^2 - z} \\ z = \bar{y}(\xi) T_a + Z_w \end{pmatrix}, \quad (8)$$

$$N_0(\xi) = \begin{pmatrix} \frac{\partial x}{\partial \eta} = \frac{S_1}{2} \bar{x}(\xi) \\ \frac{\partial x}{\partial \eta} = -S_1 \\ \frac{\partial z}{\partial \eta} = 0 \end{pmatrix}, \quad N_1(\xi) = \begin{pmatrix} \frac{\partial x}{\partial \eta} = S_2 \sin(\pi \xi) \bar{y}'(\xi) \\ \frac{\partial y}{\partial \eta} = \frac{1}{y} \left(\frac{\partial x}{\partial \xi} r(\xi) + z \frac{\partial z}{\partial \eta} \right) \\ \frac{\partial z}{\partial \eta} = -S_2 \sin(\pi \xi) \frac{\partial \bar{x}}{\partial \xi} \end{pmatrix} \quad (9)$$

where $X_c, R_0, H_1, Z_c, B_w, C, X_w, r(\xi), T_a, Z_w$ are engineering (or geometric) parameters for the inboard wing, $\bar{x}(\xi)$ and $\bar{y}(\xi)$ are functions determined by the engineering parameters (such as wing section cord length, maximum camber location, etc), and S_1, S_2 determine how smooth the inboard wing section blends into the outboard wing section and the fuselage, respectively.

One application of the RAPID prototyping model is to modify the engineering parameters of an existing design to obtain an optimized design. For this purpose, one has to recover the engineering parameters from a surface grid of an existing design (a REVERSE ENGINEERING PROCESS) and then to go through a multidisciplinary design optimization process to get a better design. In this case, the reverse engineering process can also be thought of as a systems identification or least squares problem involving (airplane) geometry.

In order to make the reverse engineering possible, we first derived the canonical basis for the Hermite interpolation problems involved in the process:

$$\begin{aligned} f_{0,1}(\eta) &= (\eta - 1)^2(1 + 2\eta), \quad f_{0,2}(\eta) = \eta^2(3 - 2\eta), \\ f_{0,3}(\eta) &= \eta(\eta - 1)^2, \quad f_{0,4}(\eta) = \eta^2(\eta - 1), \\ f_{n,1}(\eta) &= (1 - \eta)e^{an\eta} + \frac{p_n}{d_n}(1 - \eta) \sinh(an\eta) + \frac{q_n}{d_n} \eta \sinh(an(1 - \eta)), \\ f_{n,2}(\eta) &= \eta e^{an(1-\eta)} + \frac{q_n}{d_n}(1 - \eta) \sinh(an\eta) + \frac{p_n}{d_n} \eta \sinh(an(1 - \eta)), \end{aligned}$$

$$f_{n,3}(\eta) = -\frac{an}{d_n}(1-\eta)\sinh(an\eta) + \frac{\sinh(an)}{d_n}\eta\sinh(an(1-\eta)),$$

$$f_{n,4}(\eta) = -\frac{\sinh(an)}{d_n}(1-\eta)\sinh(an\eta) + \frac{an}{d_n}\eta\sinh(an(1-\eta)),$$

where $n = 1, 2, \dots$ and

$$d_n := \sinh^2(an) - (an)^2,$$

$$p_n := an(an-1) - \sinh(an)e^{an},$$

$$q_n := ane^{an} - (an-1)\sinh(an).$$

Then we used the following reverse engineering model for surfaces generated by (4)–(7):

$$\begin{aligned} F(\xi, \eta) := & \left(a_0^{(1)} f_{0,1}(\eta) + a_0^{(2)} f_{0,2}(\eta) + a_0^{(3)} f_{0,3}(\eta) + a_0^{(4)} f_{0,4}(\eta) \right) \\ & + \sum_{n=1}^m \left(\left(a_n^{(1)} f_{n,1}(\eta) + a_n^{(2)} f_{n,2}(\eta) + a_n^{(3)} f_{n,3}(\eta) + a_n^{(4)} f_{n,4}(\eta) \right) \cos(2n\pi\xi) \right. \\ & \left. + \left(b_n^{(1)} f_{n,1}(\eta) + b_n^{(2)} f_{n,2}(\eta) + b_n^{(3)} f_{n,3}(\eta) + b_n^{(4)} f_{n,4}(\eta) \right) \sin(2n\pi\xi) \right) \\ & + \left(B_0(\xi) - a_0^{(1)} - \sum_{n=1}^m \left(a_n^{(1)} \cos(2n\pi\xi) + b_n^{(1)} \sin(2n\pi\xi) \right) \right) f_{m+1,1}(\eta) \\ & + \left(B_1(\xi) - a_0^{(2)} - \sum_{n=1}^m \left(a_n^{(2)} \cos(2n\pi\xi) + b_n^{(2)} \sin(2n\pi\xi) \right) \right) f_{m+1,2}(\eta) \\ & + \left(N_0(\xi) - a_0^{(3)} - \sum_{n=1}^m \left(a_n^{(3)} \cos(2n\pi\xi) + b_n^{(3)} \sin(2n\pi\xi) \right) \right) f_{m+1,3}(\eta) \\ & + \left(N_1(\xi) - a_0^{(4)} - \sum_{n=1}^m \left(a_n^{(4)} \cos(2n\pi\xi) + b_n^{(4)} \sin(2n\pi\xi) \right) \right) f_{m+1,4}(\eta). \end{aligned}$$

For example, the corresponding reverse engineering process for the inboard wing section can be summarized in the following algorithm.

Algorithm 1 For a given wing surface grid $\{F_{i,j} : 1 \leq i \leq k, 1 \leq j \leq l\}$ with $i = 1, k$ corresponding to the inboard/outboard wing intersection and the wing/fuselage intersection, respectively, recover the engineering parameters for the inboard wing section as follows.

Step 1. Use $\{F_{1,j} : 1 \leq j \leq l\}$ to recover $B_0(\xi)$ as given in (8) (i.e., recover the engineering parameters for the inboard/outboard wing intersection).

Step 2. Use $\{F_{k,j} : 1 \leq j \leq l\}$ to recover $B_1(\xi)$ as given in (8) (i.e., recover the engineering parameters for the wing/fuselage intersection).

Step 3. Estimate the parameters ξ_1, \dots, ξ_k and η_1, \dots, η_l corresponding to the surface grid (i.e., determine the original grid distribution used to generate the surface grid).

Step 4. Recover the Neumann boundary conditions (i.e., S_1, S_2) by using the x -components $\{x_{i,j}\}$ of the surface grid; i.e., find S_1, S_2 by solving the following overdetermined system of linear equations with unknowns $a_n^{(1)}, a_n^{(2)}, a_n^{(3)}, a_n^{(4)}, b_n^{(1)}, b_n^{(2)}, b_n^{(3)}, b_n^{(4)}, S_1, S_2$:

$$\begin{aligned} v_1^{i,j} S_1 + v_2^{i,j} S_2 + \sum_{n=0}^m \left(g_{n,1}^{i,j} a_n^{(1)} + g_{n,2}^{i,j} a_n^{(2)} + g_{n,3}^{i,j} a_n^{(3)} + g_{n,4}^{i,j} a_n^{(4)} \right) \\ + \sum_{n=1}^m \left(h_{n,1}^{i,j} b_n^{(1)} + h_{n,2}^{i,j} b_n^{(2)} + h_{n,3}^{i,j} b_n^{(3)} + h_{n,4}^{i,j} b_n^{(4)} \right) = \gamma_{i,j}, \end{aligned}$$

for $1 \leq i \leq k, 1 \leq j \leq l$,

where $v_1^{i,j}, v_2^{i,j}, g_{n,1}^{i,j}, g_{n,2}^{i,j}, g_{n,3}^{i,j}, g_{n,4}^{i,j}, h_{n,1}^{i,j}, h_{n,2}^{i,j}, h_{n,3}^{i,j}, h_{n,4}^{i,j}, \gamma_{i,j}$ are constants given by the following formulas:

$$\begin{aligned} v_1^{i,j} &= \frac{1}{2} \bar{x}(\xi_i) f_{m+1,3}(\eta_j), \\ v_2^{i,j} &= \sin(\pi \xi_i) \bar{y}'(\xi_i) f_{m+1,4}(\eta_j), \\ g_{n,r}^{i,j} &= (f_{n,r}(\eta_j) - f_{m+1,r}(\eta_j)) \cos(2\pi n \xi_i), \\ h_{n,r}^{i,j} &= (f_{n,r}(\eta_j) - f_{m+1,r}(\eta_j)) \sin(2\pi n \xi_i), \\ \gamma_{i,j} &= x_{i,j} - (\bar{x}(\xi_i) + X_c) f_{m+1,1}(\eta_j) - \left(\frac{B_w}{C} \bar{x}(\xi_i) + X_w \right) f_{m+1,2}(\eta_j). \end{aligned}$$

With the above algorithm, we can recover the engineering parameters of the inboard wing section with error less than 0.1% for a surface grid generated by the PDE model (cf. Figure 1 for original surface grids of the fuselage and wing and Figure 2 for the surface grids generated by the recovered engineering parameters).

2.3 Conclusions

The current reverse engineering model can be used for the following wing configuration:

- high wing low aspect ratio short fuselage,
- double-delta transport with low wing,
- HSCT type configuration,
- Delta wing configuration.

Another direction is to measure an existing wing tunnel model using a laser digitizer and apply the reverse engineering model to the digitized surface points to recover the engineering parameters according to the RAPID model. The mathematical problems involved are the following:

- automatic identification of boundary points,
- parametrization of data points based on boundary curves.

The first problem is to build a mathematical model that can “realize the human perception of boundary points of a surface grid”. This is more or less a mathematical modeling problem in artificial intelligence. We shall use concepts and ideas in the projective geometry to find a reasonable solution. The second problem is related to accuracy and stability of a free form surface fitting of a data cloud. We will study the potential of the inverse of Coons mapping for finding a reliable parametrization of data points. This is a very difficult issue. Note that, in Algorithm 1, we had to rely on the special structure of the underlying model to find ξ_i, η_j in Step 3, which is the main source of errors in our reverse engineering process. Major progress in this direction will be beneficial not only to Air Force, but also to the whole aerospace industry.

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3 Robust Regression and Huber M-Estimator

Relationships between a linear ℓ_1 estimation problem and the Huber M-estimator problem can be easily established by their dual formulations. The least norm solution of a linear programming problem studied by Mangasarian and Meyer provides a key link between the dual problems. Based on the dual formulations, we establish a local linearity property of the Huber M-estimators with respect to the tuning parameter γ and derive that the solution set of the Huber M-estimator problem is Lipschitz continuous with respect to perturbations of the tuning parameter γ . As a consequence, the set of the linear ℓ_1 estimators is the limit of the set of the Huber M-estimators as $\gamma \rightarrow 0^+$. Thus, the Huber M-estimator problem has many solutions for small tuning parameter γ if the linear ℓ_1 estimation problem has multiple solutions. A recursive version of Madsen and Nielsen's algorithm based on computation of the Huber M-estimator is proposed for finding a linear ℓ_1 estimator. This part is a summary of a joint paper written by J. Swetits and the principle investigator [16].

3.1 Review on ℓ_1 Regression and Huber M-estimator

Consider the following linear ℓ_1 estimation problem of finding a vector x^* in \mathbb{R}^n that solves the following minimization problem:

$$\min_x \|Ax - d\|_1, \quad (10)$$

where A is $m \times n$ ($m > n$) representing the underlying linear model, x in \mathbb{R}^n is the parameter vector, $d \in \mathbb{R}^m$ is the data vector, and $\|z\|_1 := \sum_{i=1}^m |z_i|$ is the ℓ_1 -norm of z . In general, one might assume that A has rank n so that different parameter vectors correspond to different regression functions, even though this assumption is not required in our study of (10).

The linear ℓ_1 estimation problem is much more difficult to solve than the linear maximum likelihood estimation problem, where the ℓ_2 -norm, $\|z\|_2 := (\sum_{i=1}^m z_i^2)^{\frac{1}{2}}$, is used instead of the ℓ_1 -norm. See [1, 2, 3, 7, 18, 25, 27, 29, 30] for various algorithms for solving the linear ℓ_1 estimation problem. One reason for solving (10) instead of the corresponding least squares problem is that linear ℓ_1 estimators are more robust than linear least squares estimators [9, 10] in the presence of outliers. Note that (10) is referred as a nonsmooth optimization problem because the objective function (*i.e.*, the expression one tries to minimize) is not a differentiable function of parameters x_1, \dots, x_n . Many robust regression models allow one to get a robust estimator without involving nonsmooth optimization problems [10]. The most well-known one is the Huber M-estimator problem that combines the robustness of the linear ℓ_1 regression model with the smoothness of the linear maximum likelihood regression model by using the Huber's cost function, depending on a given tuning constant $\gamma > 0$, defined by

$$\rho(t) = \begin{cases} \frac{1}{2}t^2, & \text{if } |t| \leq \gamma \\ \gamma|t| - \frac{1}{2}\gamma^2, & \text{otherwise.} \end{cases}$$

The Huber M-estimator problem is to find a vector x^* in \mathbb{R}^n such that x^* solves the following minimization problem:

$$\min_x \sum_{i=1}^m \rho[(Ax - d)_i], \quad (11)$$

where $(Ax - d)_i$ denotes the i^{th} component of the vector. In general, there is a scaling parameter τ involved in the Huber M-estimator problem. For convenience, we assume that $\tau \equiv 1$. Note that Huber's cost function is

a convex differentiable piecewise quadratic polynomial and the objective function in (11) is differentiable. The purpose of Huber's cost function is to measure $(Ax - d)_i$ by $(Ax - d)_i^2$ (as in maximum likelihood estimation) when $(Ax - d)_i$ is "relatively small" while it measures $(Ax - d)_i$ by $|(Ax - d)_i|$ (as in linear ℓ_1 estimation) when d_i is an outlier (i.e., $|(Ax - d)_i|$ is "relatively large").

Recently, there have been many papers devoted to design of numerical algorithms for solving the Huber M-estimator problem [5, 6, 16, 17, 23, 28], as well as to relationships between linear ℓ_1 estimators and Huber M-estimators [4, 18, 19]. Madsen and Nielsen [18], and Madsen, Nielsen, and Pinar [19] show that algorithms for computing Huber M-estimators can also be used to find linear ℓ_1 estimators, by establishing an explicit correspondence between linear ℓ_1 estimators and Huber M-estimators. The purpose of this section is to show that more revealing relationships between linear ℓ_1 estimators and Huber M-estimators can be easily derived through dual formulations of (10) and (11). More specifically, we obtain that the dual solution of the Huber M-estimator problem is the least norm solution of the dual linear programming problem of (10) when the tuning parameter $\gamma > 0$ is small enough. The proof is based on a characterization of the least norm solution of a linear program proved by Mangasarian and Meyer [21, 20]. As consequences, we not only recover the known results about linear ℓ_1 estimators and Huber M-estimators, but also derive new ones. This allows us to explicitly verify whether a given parameter γ is small enough to produce a linear ℓ_1 estimator. We will propose a recursive version of Madsen and Nielsen's algorithm for finding a linear ℓ_1 estimator by solving the corresponding Huber M-estimator problem.

It is well-known that either (10) or (11) may have infinitely many solutions. Sufficient conditions for uniqueness of the linear ℓ_1 estimator and the Huber M-estimator are given in [4, 17, 18, 19]. However, it is not clear whether there is a connection between the uniqueness of the linear ℓ_1 estimator and the Huber M-estimator. We show that the uniqueness of the Huber M-estimator for every small tuning factor γ implies the uniqueness of the linear ℓ_1 estimator. However, a counterexample shows that the converse does not hold. That is, there exist A and d such that (10) has a unique solution, but the corresponding Huber M-estimator problem (11) has infinitely many solutions for every $0 < \gamma \leq \delta$, where δ is a positive constant.

The section is organized as follows. Dual problems of (10) and (11) are given in Subsection 3.2 and characterizations of solutions of (10) and (11) are also given in terms of their dual solutions, respectively. In Subsection 3.3, we

first give the Lipschitz stability of X^γ with respect to the perturbations of γ . Then, based on the dual characterizations given in the previous subsection, we establish a local linearity property of the solution set X^γ of (11) as a set-valued mapping of the parameter γ when $\gamma > 0$ is small enough. Moreover, we obtain that the uniqueness of the Huber M-estimator for small positive tuning parameter γ implies the uniqueness of the linear ℓ_1 estimator. The converse is also true under the nondegeneracy assumption on the least norm solution of a dual problem of (10). But the converse is not true in general. We give an example of the linear ℓ_1 estimation problem which has a unique solution, but the corresponding Huber M-estimator problem (11) does have infinitely many solutions for $0 < \gamma \leq \delta$ with some positive constant δ . In Subsection 3.4, a recursive algorithm for finding a linear ℓ_1 estimator is proposed. The algorithm allows one to explicitly construct a solution of (10) by solving finitely many Huber M-estimator problems. Conclusions are included in Subsection 3.5.

To conclude the subsection we give some notations used in this section. If A is a matrix and x is a (column) vector, A_i denotes the i^{th} row of A and x_i denotes the i^{th} component of x . (Note $A_i x \equiv (Ax)_i$.) For a vector x (or a matrix A), x^T (or A^T) is its transpose. For two vectors x and y , $x \leq y$ means $x_i \leq y_i$ for every index i . For convenience, when x is a vector and α is a number, $x \leq \alpha$ denotes $x_i \leq \alpha$ for every index i . We use $z_{-\gamma}^\gamma$ to denote the vector whose i^{th} component is $\max\{-\gamma, \min\{\gamma, z_i\}\}$. The ℓ_∞ -norm, $\|\cdot\|_\infty$, of a vector $z \in \mathbb{R}^m$ is $\|z\|_\infty = \max_{1 \leq i \leq m} |z_i|$. The set of all solutions of (10) is denoted by X^0 , while the set of all solutions of (11) is denoted by X^γ for any given tuning parameter γ . The null space of a matrix A is defined as $\{x \in \mathbb{R}^n : Ax = 0\}$.

3.2 Dual Formulations

In this subsection we give the dual formulations of (10) and (11) as a linear programming problem and a quadratic programming problem, respectively. These dual formulations provide characterizations of linear ℓ_1 estimators and Huber M-estimators in terms of their dual solutions. Then, from Mangasarian and Meyer's characterization of the least norm solution of a linear program [21, 20], we know that the unique dual solution of (11) is actually the least norm dual solution of (10) when $\gamma > 0$ is small enough.

Consider the following dual formulation of (10):

$$\min_y d^T y \quad \text{subject to } A^T y = 0, \quad -1 \leq y \leq 1. \quad (12)$$

The following lemma is essentially known, but the form of the statement given here is more convenient for our purposes. For another form of the lemma, see [24, 19].

Lemma 2 *Let $\bar{x} \in \mathbb{R}^n$ and $\bar{y} \in \mathbb{R}^m$. Then \bar{x} and \bar{y} are solutions of (10) and (12), respectively, if and only if the following conditions hold:*

$$\begin{aligned} A^T \bar{y} &= 0, \quad -1 \leq \bar{y}_i \leq 1, \\ (A\bar{x} - d)_i &\geq 0, \quad \text{if } \bar{y}_i = 1, \\ (A\bar{x} - d)_i &\leq 0, \quad \text{if } \bar{y}_i = -1, \\ (A\bar{x} - d)_i &= 0, \quad \text{if } -1 < \bar{y}_i < 1. \end{aligned} \tag{13}$$

Note that the standard KKT-conditions for (12) involve a multiplier \bar{z} for the constraints $-1 \leq y \leq 1$ and an equation $d - A\bar{x} - \bar{z} = 0$. Here we use $\bar{z} := -(A\bar{x} - d)$ to eliminate \bar{z} in the above lemma. The following characterization of linear ℓ_1 estimators based on a solution to (12) follows immediately from Lemma 2.

Corollary 3 *Let y^* be a solution of (12). Then \bar{x} is a solution of (10) if and only if \bar{x} satisfies the following conditions:*

$$\begin{aligned} (A\bar{x} - d)_i &\geq 0, \quad \text{if } y_i^* = 1, \\ (A\bar{x} - d)_i &\leq 0, \quad \text{if } y_i^* = -1, \\ (A\bar{x} - d)_i &= 0, \quad \text{if } -1 < y_i^* < 1. \end{aligned} \tag{14}$$

The classical approximation theoretic characterization of solutions to (10) states that $\bar{x} \in \mathbb{R}^n$ solves (10) if and only if there exists $\bar{y} \in \mathbb{R}^m$ such that $-1 \leq \bar{y}_i \leq 1$, $A^T \bar{y} = 0$, and $\bar{y}^T (A\bar{x} - d) = \|A\bar{x} - d\|_1$ (cf. [29, Chapter 6]). It is easy to see that these conditions are equivalent to (13) or (14).

Now consider the least norm solution of (12), which is the unique solution of the following quadratic program:

$$\min_y d^T y + \frac{\epsilon}{2} \|y\|_2^2 \quad \text{subject to } A^T y = 0, -1 \leq y_i \leq 1, \tag{15}$$

when $\epsilon > 0$ is sufficiently small, as shown in the following lemma by Mangasarian and Meyer [21, 20].

Lemma 4 *Let y^ϵ be the unique solution of the strictly convex quadratic program (15). Then there exists $\delta > 0$ such that y^ϵ is the least norm solution of (12) for $0 < \epsilon < \delta$.*

Here we say that y^* is the least norm solution of (12) if y^* is the solution of the following strictly convex quadratic programming problem:

$$\min_{y \in Y^*} \frac{1}{2} \|y\|_2^2,$$

where Y^* is the set of all solutions to (12). That is, y^* is the least norm solution of (12) if y^* is the solution of (12) that has the smallest ℓ_2 -norm. The least norm solution of (12) is actually the unique common solution of (12) and (15).

Lemma 5 *If the solution y^* of (15) is also a solution of (12), then y^* is the least norm solution of (12).*

Since $\rho'(t) = (t)_{-\epsilon}^\epsilon$, the gradient of the objective function in (11) is $A^T(Ax - d)_{-\epsilon}^\epsilon$. Since (11) is a convex differentiable optimization problem, x^* is a solution of (11) if and only if x^* is a zero of the gradient of the objective function; i.e., x^* is a solution of the following system of piecewise linear equations:

$$A^T(Ax - d)_{-\epsilon}^\epsilon = 0. \quad (16)$$

For easy reference, we give the following lemma for the equivalence of (16) and (11).

Lemma 6 *A vector x^γ is a solution of (16) if and only if x^γ is a solution of (11).*

It is known that (16) can be considered as a dual problem of (15) [17, 23]. Therefore, (11) and (15) are dual problems. Here is the relation between solutions of (15) and (11) [17].

Lemma 7 *A vector y^ϵ is the solution of (15) if and only if $y^\epsilon = \frac{1}{\epsilon}(Ax^\epsilon - d)_{-\epsilon}^\epsilon$, where x^ϵ is a solution of (11).*

Therefore, in order to get the solution of (15), one only needs to find a Huber M-estimator by solving (11) (or (16)). Many algorithms (including Newton methods, matrix splitting methods, conjugate gradient methods) were developed for solving the quadratic program (15) by exploring its dual structure (16) [17, 23, 14].

For a better understanding of the duality between (11) and (15), we recast Lemma 7 as follows.

Lemma 8 *Let $\bar{x} \in \mathbb{R}^n$ and $\bar{y} \in \mathbb{R}^m$. Then \bar{x} and \bar{y} are solutions of (11) and (15), respectively, if and only if the following conditions hold:*

$$\begin{aligned} A^T \bar{y} &= 0, \quad -1 \leq \bar{y} \leq 1, \\ (A\bar{x} - d)_i &\geq \gamma, \quad \text{if } \bar{y}_i = 1, \\ (A\bar{x} - d)_i &\leq -\gamma, \quad \text{if } \bar{y}_i = -1, \\ (A\bar{x} - d)_i &= \gamma \bar{y}_i, \quad \text{if } -1 < \bar{y}_i < 1. \end{aligned} \tag{17}$$

Note that the standard KKT-conditions for (15) involve a multiplier \bar{z} for the constraints $-1 \leq y \leq 1$ and an equation $d - \epsilon \bar{y} - A\bar{x} - \bar{z} = 0$. Here we use $\bar{z} := -(A\bar{x} - d - \epsilon \bar{y})$ to eliminate \bar{z} in the above lemma. The following characterization of the Huber M-estimators based on a solution to (12) follows immediately from Lemma 8.

Corollary 9 *Let y^* be a solution of (15). Then \bar{x} is a solution of (11) if and only if \bar{x} satisfies the following conditions:*

$$\begin{aligned} (A\bar{x} - d)_i &\geq \gamma, \quad \text{if } y_i^* = 1, \\ (A\bar{x} - d)_i &\leq -\gamma, \quad \text{if } y_i^* = -1, \\ (A\bar{x} - d)_i &= \gamma y_i^*, \quad \text{if } -1 < y_i^* < 1. \end{aligned} \tag{18}$$

Lemma 5 provides a way to verify whether or not the solution of (15) is the least norm solution of (12). By Lemma 4, there exists a positive constant δ such that the solution of (15) is the least norm solution y^* of (12) for $0 < \gamma \leq \delta$. But we do not know how small δ should be. The following lemma tells us that if the solution of (15) is the least norm solution y^* for some $\gamma = \delta > 0$, then y^* is also the solution of (15) for any $0 < \gamma < \delta$.

Lemma 10 *If the solution y^δ of (15) is the least norm solution y^* of (12) for some $\gamma = \delta > 0$, then the solution y^γ of (15) is the least norm solution of (12) for any $0 < \gamma \leq \delta$ (i.e., $y^\gamma \equiv y^*$ for $0 < \gamma \leq \delta$).*

The above lemma should be compared with Lemma 3 and Theorem 4 of [19] wherein results are formulated in terms of a “sign vector” associated with solutions to (16). The sign vector s^γ is related to y^γ as follows: $s_i^\gamma = y_i^\gamma$ if $|y_i^\gamma| = 1$ and $s_i^\gamma = 0$ if $|y_i^\gamma| < 1$. Madsen, Nielsen, and Pinar [19] proved that $s^\gamma \equiv s^\delta$ for $0 < \gamma < \delta$ if $\delta > 0$ is small enough.

3.3 Linear ℓ_1 Estimator and Huber M-Estimator

By Hoffman's error bound for approximate solutions of a system of linear equalities and inequalities, we obtain the Lipschitz stability of X^γ with respect to γ . By using the dual characterizations given in Lemmas 3 and 9, as well as Lemma 4, we show that the solution set X^γ of (11) is a linear mapping of the parameter γ when $\gamma > 0$ is small enough. Moreover, we obtain that the uniqueness of the Huber M-estimator for small positive tuning parameter γ implies the uniqueness of the linear ℓ_1 estimator. The converse is also true under the nondegeneracy assumption on the least norm solution of (12). But the converse is not true in general. We give an example of the linear ℓ_1 problem which has a unique solution, but the corresponding Huber M-estimator problem (11) does have infinitely many solutions for $0 < \gamma \leq \delta$ with some positive constant δ . Our example is based on a new explicit characterization of the least norm solution of (12).

First, we show the Lipschitz stability of Huber M-estimators with respect to the perturbations of γ . Let X^ϵ be the solution set of (11) and X^0 be the solution set of (10).

Theorem 11 *Let $\delta > 0$ be such that the solution of (15) for $\gamma = \delta$ is the least norm solution y^* of (12). Then there exists a positive constant λ such that*

$$H(X^{\bar{\gamma}}, X^\epsilon) \leq \lambda \cdot \epsilon \quad \text{for } 0 \leq \gamma, \bar{\gamma} \leq \delta, \quad (19)$$

where $H(X, Y)$ is the Hausdorff distance between X and Y defined as

$$H(X, Y) := \max \left\{ \max_{x \in X} \min_{y \in Y} \|x - y\|_2, \max_{y \in Y} \min_{x \in X} \|y - x\|_2 \right\}.$$

Note that the above theorem shows that, for small ϵ , a Huber M-estimator is almost the same as a linear ℓ_1 estimator in the sense that the difference is a constant multiple of ϵ .

Various relations between X^ϵ and X^0 were given by Madsen, Nielsen, and Pinar [19]. However, these relations involve a sign pattern of certain vectors. Here we give a pure algebraic relation between X^γ and X^0 .

Theorem 12 *Suppose that the solution of (15) for some $\gamma = \delta$ is the least norm solution y^* of (12). Then*

$$X^\tau \supset \frac{\tau - \alpha}{\beta - \alpha} X^\beta + \frac{\beta - \tau}{\beta - \alpha} X^\alpha \quad \text{for } 0 \leq \alpha < \tau < \beta \leq \delta, \quad (20)$$

where $\mu X + \nu Y := \{\mu x + \nu y : x \in X, y \in Y\}$.

The above theorem shows that X^γ is a convex set-valued mapping of γ for $0 \leq \gamma \leq \delta$. One important technical aspect of the above theorem is that we "know" how small δ should be. However, X^γ is actually a linear set-valued mapping of γ for $\gamma > 0$ small enough. The drawback of the next theorem is that there is no criterion to identify how small the γ 's should be.

Theorem 13 *If the columns of A are linearly independent (i.e., the rank of A is n), then there exists a positive constant ϵ such that*

$$X^\tau = \frac{\tau - \alpha}{\beta - \alpha} X^\beta + \frac{\beta - \tau}{\beta - \alpha} X^\alpha \quad \text{for } 0 \leq \alpha < \tau < \beta \leq \epsilon. \quad (21)$$

Let $\alpha = 0$, $\beta = \delta$, and $0 < \tau < \delta$ in Theorem 12. By (20), we have $X^\tau \supset \frac{\tau}{\delta} X^\delta + (1 - \frac{\tau}{\delta}) X^0$. If $X^\tau = \{x^\tau\}$ has only one element, then $X^0 = \{x^0\}$ and $X^\delta = \{x^\delta\}$ are both singletons. Moreover, $x^\tau = \frac{\tau}{\delta} x^\delta + (1 - \frac{\tau}{\delta}) x^0$. That is, x^τ is a linear function of τ for $0 \leq \tau \leq \delta$. Thus, we have the following consequence of Theorem 12.

Theorem 14 *Suppose that the solution of (15) for some $\gamma = \delta$ is the least norm solution of (12). If the Huber M-estimator problem (11) has a unique solution x^γ for $\gamma > 0$ small enough, then the linear ℓ_1 estimation problem (10) has a unique solution x^0 . Moreover, $x^\gamma = \frac{\gamma}{\delta} x^\delta + (1 - \frac{\gamma}{\delta}) x^0$ is a linear function of γ for $0 \leq \gamma \leq \delta$.*

It is interesting to see that $x^0 = \frac{\delta}{\delta - \gamma} x^\gamma - \frac{\gamma}{\delta - \gamma} x^\delta$ for $0 < \gamma < \delta$. That is, we can find the unique linear ℓ_1 estimator by two Huber M-estimators of different small tuning parameters.

The converse of the above theorem about the uniqueness is also true if the least norm solution of (12) is nondegenerate. A solution y^* of (12) is said to be nondegenerate if there exists a solution \bar{x} of (10) such that

$$\begin{aligned} (A\bar{x} - d)_i &> 0, \text{ if } y_i^* = 1, \\ (A\bar{x} - d)_i &< 0, \text{ if } y_i^* = -1, \\ (A\bar{x} - d)_i &= 0, \text{ if } -1 < y_i^* < 1. \end{aligned} \quad (22)$$

Theorem 15 *Suppose that the least norm solution of (12) is nondegenerate and the linear ℓ_1 estimation problem (10) has a unique solution. Then there exists $\delta > 0$ such that the Huber M-estimator problem (11) has a unique solution x^ϵ for $0 < \epsilon < \delta$. Moreover, $\Phi(x)$ is actually a strictly convex quadratic function in a neighborhood of x^γ for $0 < \gamma \leq \delta$ and $\Phi(x)$ is*

twice differentiable at x^ϵ (i.e., the Hessian $\Phi''(x^\epsilon)$ exists), where $\Phi(x)$ is the objective function in (11); i.e.,

$$\Phi(x) = \sum_{i=1}^m \rho[(Ax - d)_i].$$

Remark. Let y^γ be the solution of (15) and $W(\gamma)$ be the diagonal matrix whose i^{th} diagonal entry is 1 if $-1 < y_i^\gamma < 1$ and 0 otherwise. Since $W(\gamma)Az = 0$ has a unique solution $z^* = 0$ whenever $A^T W(\gamma)A$ is nonsingular, the above proof implies that (11) has a unique solution if $A^T W(\gamma)A$ is nonsingular. This sufficient condition for uniqueness of the Huber M-estimator was observed by many authors [4, 17, 18, 19].

However, the above theorem is not true without the nondegeneracy assumption. To construct a counterexample, we need the following explicit characterization of the least norm solution of (12).

Theorem 16 *Let $\varphi \in \mathbb{R}^m$ be such that $\varphi^T A = 0$, $\max_{1 \leq i \leq m} |\varphi_i| = 1$, and there exists a positive constant δ such that, for $0 < \gamma \leq \delta$,*

$$X^\gamma(\varphi) := \left\{ x \in \mathbb{R}^n : \begin{array}{l} \varphi_i(Ax - d)_i \geq \gamma \text{ if } |\varphi_i| = 1, \\ (Ax - d)_i = \varphi_i \gamma \text{ if } |\varphi_i| < 1 \end{array} \right\} \neq \emptyset.$$

Then φ is the least norm solution of (12) and $X^\gamma(\varphi) \equiv X^\gamma$ for $0 < \gamma \leq \delta$.

One can construct an example showing that the least norm solution φ of (12) is degenerate, even though (12) has nondegenerate solutions. In the case that $\alpha = 0$, the Huber M-estimator problem (11) also has a unique solution x^γ with $x_1^\gamma = 0$ and $x_2^\gamma = \frac{\gamma}{4}$ for small γ , despite the degeneracy of the least norm solution φ . Therefore, the nondegeneracy assumption in Theorem 15 is not necessary for the uniqueness of the Huber M-estimator.

3.4 Computation of A Linear ℓ_1 Estimator

In [18], Madsen and Nielsen proposed to compute a sign pattern vector s for the linear ℓ_1 estimation problem (10) by solving (11) for very small tuning parameter γ . Then, by solving a system of linear inequalities and equalities, a linear ℓ_1 estimator can be obtained. In this subsection we propose a recursive version of Madsen and Nielsen's algorithm for finding a linear ℓ_1 estimator. By the dual relationships given in Subsection 3.2, we know exactly how small γ should be in computation. Moreover, unlike Madsen

and Nielsen's approach, a linear ℓ_1 estimator is explicitly constructed by using Huber M-estimators.

First let us explain Madsen and Nielsen's method for computing a linear ℓ_1 estimator by solving Huber M-estimator problems. Suppose that we have a solution x^γ of (16) (or (11)) for some very small γ . By Lemma 7, $y^\gamma = \frac{1}{\gamma}(Ax^\gamma - d)_{-}^\gamma$ is a solution of (15). Then, by Lemma 4, y^γ is the least norm solution of (12). By Corollary 3, one can get a linear ℓ_1 estimator by solving the feasibility problem (14), a system of linear inequalities and equalities with $y^* \equiv y^\gamma$.

In general, a system of linear inequalities and equalities is not trivial to solve. However, under the assumption of nonsingularity of a certain matrix, (14) is reduced to a system of linear equations. More specifically, let $W(\epsilon)$ be the $m \times m$ diagonal matrix whose i^{th} diagonal entry is 1 if $|y_i^\epsilon| < 1$ and 0 if $|y_i^\epsilon| = 1$. By Lemma 4, there exists a positive number δ such that $y^\epsilon \equiv y^0$, the least norm solution of (12), for $0 < \epsilon < \delta$. As a result, $W(\epsilon) \equiv W(0)$ is a constant matrix for $0 < \epsilon < \delta$. If $A^T W(\epsilon) A$ is nonsingular, then the unique solution of (14) can be found by solving a system of linear equations as shown in the following theorem.

Lemma 17 *Let $\delta > 0$ be such that the solution y^δ of (15) (with $\gamma = \delta$) is the least norm solution of (12), and let $W(\delta)$ be the $m \times m$ diagonal matrix whose i^{th} diagonal entry is 1 if $|y_i^\delta| < 1$ and 0 if $|y_i^\delta| = 1$. If $A^T W(\delta) A$ is nonsingular, then the Huber M-estimator problem (11) has a unique solution x^ϵ for $0 < \epsilon < \delta$ and*

$$x^\epsilon = x^\delta + (\epsilon - \delta)z^0, \quad (23)$$

where z^0 is the unique solution of the following linear system:

$$W(\delta)Az = W(\delta)y^\delta. \quad (24)$$

Moreover, the linear ℓ_1 estimation problem (10) has a unique solution $x^0 = x^\delta - \delta z^0$, which is also the unique solution of the following linear system:

$$W(\delta)Ax = W(\delta)d. \quad (25)$$

In general, from (14), we know that all solutions of (10) are in the set

$$X(y^\gamma) := \{x \in \mathbb{R}^n : (Ax - d)_i = 0 \text{ if } |y_i^\gamma| < 1\}.$$

Therefore, we consider the following minimization problem:

$$\min_{x \in X(y^\gamma)} \sum_{i=1}^m \rho[(Ax - d)_i], \quad (26)$$

which is equivalent to a system of piecewise linear equations similar to (16):

$$\bar{A}^T(\bar{A}\bar{x} - \bar{d})_{-\gamma}^\gamma = 0, \quad (27)$$

where $x = x^\gamma + T\bar{x}$, T is a transformation matrix with appropriate order, and $\bar{x} \in \mathbb{R}^{\bar{n}}$ with $\bar{n} < n$. Now we consider that (27) is the Huber M-estimator problem (cf. (16)) corresponding to a “simpler” linear ℓ_1 estimation problem and try to find a solution of the new linear ℓ_1 estimation problem. One important relation between these two ℓ_1 estimation problems is that if \bar{x}^* is a solution of the new ℓ_1 estimation problem, then $x^* = x^\gamma + T\bar{x}^*$ is a solution of the original ℓ_1 estimation problem. Therefore, the problem is reduced to finding a solution of a “simpler” problem. After repeating this process a few times, we see that the condition in Lemma 17 will be satisfied for the final Huber M-estimator problem and then we can get a solution of the final linear ℓ_1 estimation problem by solving a system of linear equations. By doing so, we can explicitly construct a linear ℓ_1 estimator of (10) by using the Huber M-estimators and transformation matrices obtained in the process.

The above recursive method of computing a linear ℓ_1 estimator is formulated in the following algorithm.

Algorithm 18 Let $k = 0$, $T^0 = I$ (the $n \times n$ identity matrix), $d^0 = d$, $x^0 = 0$, and $A^0 = A$. Compute a solution of (10) as follows:

Step 1. find $\epsilon > 0$ and a solution u^k of

$$(A^k)^T (A^k u^k - d^k)_{-\epsilon}^\epsilon = 0 \quad (28)$$

such that $v^k := \frac{1}{\epsilon}(A^k u^k - d^k)_{-\epsilon}^\epsilon$ is a solution of

$$\min_v (d^k)^T v \quad \text{subject to} \quad (A^k)^T v = 0, -1 \leq v \leq 1; \quad (29)$$

Step 2. let W^k be the diagonal matrix whose i^{th} diagonal entry is 1 if $|v_i^k| < 1$ and 0 otherwise;

Step 3. if $k > 0$ and $W^k = W^{k-1}$, let $x^{k+1} := x^k + T^k u^k$ and go to Step 9;

Step 4. find a solution z^k of the linear system

$$W^k A^k z = W^k d^k; \quad (30)$$

Step 5. let $x^{k+1} := x^k + T^k z^k$;

Step 6. if $(A^k)^T W^k A^k$ is nonsingular, then go to Step 9;

Step 7. let the columns of B^k be a basis of the null space of $W^k A^k$;

Step 8. set $A^{k+1} := A^k B^k$, $T^{k+1} = T^k B^k$, $d^{k+1} := d^k - A^k z^k$, $k := k + 1$,
and go to Step 1;

Step 9. output x^{k+1} as a solution of (10).

This algorithm finds a linear ℓ_1 estimator in finitely many iterations as shown in the following theorem.

Theorem 19 *For any A and d , Algorithm 18 finds a solution of the linear ℓ_1 regression problem (10) in finitely many iterations.*

3.5 Conclusions

We show that many new relationships between the linear ℓ_1 estimators and the Huber M-estimators can be derived once one understands that the dual solution of the Huber M-estimator problem (11) with a small tuning parameter γ is the least norm solution of the dual problem of the linear ℓ_1 estimation problem (10). The dual connection between (11) and (10) allows us to establish a set-valued version of the linearity property of the Huber M-estimator with respect to the tuning parameter γ , as well as the Lipschitz stability of the Huber M-estimators with respect to perturbations of γ . It also allows us to identify how small the tuning parameter should be in the computation of the Huber M-estimators for finding a linear ℓ_1 estimator. By exploiting the dual connection, we have an almost complete understanding of how the uniqueness of the Huber M-estimator with a small tuning parameter is related to the uniqueness of the linear ℓ_1 estimator.

Our study also provides a new interpretation of the role of the Huber M-estimator in Madsen and Nielsen's method for computing a linear ℓ_1 estimator. In the case that the least norm solution of (12) is nondegenerate, all common zero indices of the error vectors $(Ax^0 - b)$ (with x^0 in the solution set of (10)) can be identified by the Huber M-estimator with a small tuning parameter γ and a linear ℓ_1 estimator can be explicitly constructed by solving another Huber M-estimator problem. However, when the least norm solution of (12) is degenerate, we have to repeatedly solve Huber M-estimator problems in order to find the common zero indices. Therefore, we propose a recursive version of Madsen and Nielsen's method for computing a

linear ℓ_1 estimator by repeatedly solving Huber M-estimator problems. The new algorithm explicitly constructs a linear ℓ_1 estimator based on Huber M-estimators, without Madsen and Nielsen's assumption that guarantees the uniqueness of both the Huber M-estimator and the linear ℓ_1 estimator.

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4 Global Error Bounds for Quadratic Inequalities

In this section we report our study on convex differentiable inequalities and show that metric regularity and Abadie's constraint qualification are equivalent for such inequalities. For convex quadratic inequalities, we show that metric regularity, the existence of a global error bound, and Abadie's constraint qualification are mutually equivalent. As a consequence, we derive two new characterizations of weak sharp minima of a convex quadratic programming problem. This is a summary of a paper written by the principle investigator [16].

4.1 Review on Global Error Bounds

Consider a nonempty convex subset S of \mathbb{R}^n defined by the following convex inequalities:

$$g(x) \leq 0, \tag{31}$$

where $g(x)$ is a mapping from \mathbb{R}^n to \mathbb{R}^m and each component $g_i(x)$ of $g(x)$ is a convex function on \mathbb{R}^n . Most likely one has to resort to some iterative method for finding an approximate solution of (31). One important criterion for accuracy of an approximate solution x is the amount of constraint violation: $\|(g(x))_+\|$. Here z_+ is a vector whose i th component is $\max\{0, z_i\}$

and $\|\cdot\|$ denotes the 2-norm on \mathbb{R}^m (i.e., $\|x\|^2 = \sum_{i=1}^n |x_i|^2$). There are both practical and theoretical reasons for studying the following estimate of the distance from any point x in \mathbb{R}^n to the feasible set S :

$$\text{dist}(x, S) \leq \gamma \cdot \|(g(x))_+\|, \quad (32)$$

where γ is a positive constant and $\text{dist}(x, S) := \min_{y \in S} \|x - y\|$. When $g(x)$ is linear, (32) is Hoffman's error estimate for approximate solutions of a system of linear inequalities [8]. Error estimate was crucial for establishing linear convergence of various descent methods for solving linearly constrained optimization problems [19, 20, 21, 22, 23, 24, 26, 17, 11, 13, 14, 15]. From a practical point of view, (32) guarantees that the distance from an approximate solution x to S is bounded by a multiple of $\|(g(x))_+\|$, an explicit measurement of infeasibility. Roughly speaking, one might expect that $\text{dist}(x, S)$ decreases proportionally as $\|(g(x))_+\|$. However, the proportional constant γ might be large and result in an undesirable situation: $\|(g(x))_+\|$ is quite small but x might be far away from the feasible set S . This is similar to the ill-conditioning of a system of linear equations. Therefore, in order to know the accuracy of an approximate solution in terms of its distance to the feasible set, it is important to know what is the exact value of γ in estimation (32). Mangasarian defined the conditioning number of the inequality system (31) as the smallest γ for which estimation (32) holds for all x [25]. There are quite a few papers devoted to the study of the conditioning number of a system of linear equalities and inequalities [6, 27, 4, 12, 5, 9, 10].

Generally, (32) does not hold if $g(x)$ is not linear. Robinson proved that (32) holds if S is bounded and has a nonempty interior [28]. For an unbounded feasible set S , Mangasarian [25] established (32) under the assumption that $g_i(x)$ are differentiable convex functions and (31) satisfies Slater's condition (i.e., there exists a point x^* such that $g(x^*) < 0$) as well as an asymptotic constraint qualification. Auslender and Crouzeix extended both Robinson and Mangasarian's results by introducing a more general asymptotic constraint qualification that can be applied to nondifferentiable convex functions $g_i(x)$. They derived (32) under Slater's condition and their asymptotic constraint qualification [2]. However, asymptotic constraint qualifications are difficult to verify. It was not clear from Auslender and Crouzeix's result whether or not (32) holds if $g_i(x)$ are convex quadratic functions. It was proved recently by Luo and Luo [18] that (32) holds if $g_i(x)$ are convex linear/quadratic functions and there exists a feasible point x^* of (31) such that $g_i(x^*) < 0$ whenever $g_i(x)$ is not linear. That is, for convex linear/quadratic functions, (32) holds when Slater's condition holds

for nonlinear constraints. Shortly after, Pang and Wang showed that (32) might not hold for convex quadratic inequalities if Slater's condition fails [32]. They introduced an interesting concept called the degree of singularity of an inequality system and proved that, if $g_i(x)$ are convex linear/quadratic functions and the degree of singularity of (31) is d , then

$$\text{dist}(x, S) \leq \rho \cdot \left(\|(g(x))_+\| + \|(g(x))_+\|^{2^{-d}} \right) \quad \text{for } x \in \mathbb{R}^n. \quad (33)$$

They also showed by examples that the above estimate is sharp in the sense that there is a convex quadratic inequality system for each $d = 0, 1, \dots$ such that [32]

$$\sup_{x \notin S} \frac{\text{dist}(x, S)}{\|(g(x))_+\| + \|(g(x))_+\|^{2^{-d}}} > 0.$$

Note that the degree of singularity of (31) is always bounded by $(m + 1)$. Therefore, (33) always holds with $d = m + 1$ [32]. This provides a general error bound for approximate solutions of a convex quadratic inequality system, even though it might not be as sharp as one expects.

From Luo-Luo and Pang-Wang's works we can appreciate the importance of Slater's condition in error estimate (32) for approximate solutions of a convex quadratic inequality system. However, one can easily construct a convex quadratic inequality system that satisfies (32) but does not satisfy Slater's condition: $g_1(x_1, x_2) = x_1 + x_2$, $g_2(x_1, x_2) = -(x_1 + x_2)$, and $g_3(x_1, x_2) = (x_1 + x_2)^2$. (It is a trivial case since the nonlinear constraint is superfluous. For nontrivial examples, see Subsection 4.4.) This simple example raises a natural question: what is the characterization of a convex quadratic inequality system that satisfies (32)? It was this question that led us to the discovery of some intrinsic connections among several seemingly unrelated concepts: Abadie's constraint qualification, metric regularity, global error bounds, and weak sharp minimum property.

The section is organized as follows. In Subsection 4.2, we give a detailed discussion of Abadie's constraint qualification, since it plays a key role in this section. The main result in Subsection 4.3 is the equivalence of Abadie's constraint qualification and metric regularity for a differentiable convex inequality system. In Subsection 4.4, we apply this characterization of metric regularity to derive a characterization of a convex quadratic inequality system that satisfies (32): error estimate (32) holds if and only if Abadie's constraint qualification is satisfied at every feasible point. Since we can reformulate a constrained minimization problem as an inequality system, weak sharp minimum property may be considered as a weaker form of

error estimate (32). From this point of view, we establish two new characterizations of weak sharp minimum property of a convex quadratic program. Finally, conclusion is included in Subsection 4.5.

4.2 Abadie's Constraint Qualification

In this subsection, we review constraint qualifications for (31), especially, Abadie's constraint qualification. First, Abadie's constraint qualification is a representation of the tangent cone by the gradients of active constraints, which can also be described by a representation of the normal cone by the gradients of active constraints. For convex differentiable optimization problems, Abadie's constraint qualification is the weakest condition that ensures the characterization of an optimal solution by Karush-Kuhn-Tucker conditions.

For a point x in a convex set S , the normal cone of S at x is defined by

$$N(x) := \{z \in \mathbb{R}^n : z^T(y - x) \leq 0 \text{ for } y \in S\}.$$

The tangent cone $T(x)$ of S at x is the polar of the normal cone $N(x)$. That is, $y \in T(x)$ if and only if $y^T z \leq 0$ for every $z \in N(x)$. The tangent cone $T(x)$ can also be defined as the closed convex cone generated by the elements in $S - x$.

Definition 20 We say that the system (31) satisfies Abadie's constraint qualification (Abadie's CQ) $x \in S$ if $T(x) = \{y \in \mathbb{R}^n : g'_i(x)^T y \leq 0 \text{ for } i \in I\}$, where $I := \{i : g_i(x) = 0\}$ is the set of indices of active constraints at x . If Abadie's CQ holds at every point in S , then we say that (31) satisfies Abadie's CQ.

By duality, we can also use the normal cone to describe Abadie's constraint qualification.

Lemma 21 For the inequality system (31), Abadie's constraint qualification is satisfied at a point $x \in S$ if and only if the normal cone of S at x is

$$\left\{ \sum_{i \in I} \lambda_i g'_i(x) : \lambda_i \geq 0 \text{ for } i \in I \right\},$$

where $I := \{i : g_i(x) = 0\}$ is the index set of active constraints at x .

The following relation about various constraint qualifications is well-known, which implies that Abadie's constraint qualification is the weakest one among them.

Lemma 22 *Consider the following constraint qualifications at a point $x \in S$:*

(LICQ): $\{g'_i(x) : i \in I\}$ is linearly independent,

(SCQ): there exists x^* such that $g_i(x^*) < 0$ for $i = 1, \dots, m$,

(MFCQ): there exists a vector u such that $g'_i(x)^T u > 0$ for $i \in I$,

(ACQ): the tangent cone of S at x is $\{y \in \mathbb{R}^n : g'_i(x)^T y \leq 0 \text{ for } i \in I\}$,

where $I := \{i : g_i(x) = 0\}$ is the index set of active constraints at x . Then

$$(\text{LICQ}) \Rightarrow (\text{SCQ}) \Leftrightarrow (\text{MFCQ}) \Rightarrow (\text{ACQ}).$$

Now we show that Abadie's constraint qualification is the weakest condition that ensures the characterization of an optimal solution of a convex differentiable optimization problem.

Consider the inequality system (31) and the following convex program:

$$\min f(x) \quad \text{subject to } g_i(x) \leq 0 \quad \text{for } i = 1, \dots, m. \quad (34)$$

where $f(x)$ is a differentiable convex function on \mathbb{R}^n . We say that x^* is a Karush-Kuhn-Tucker point (KKT point) of (34) if there exist nonnegative scalars λ_i such that

$$f'(x^*) + \sum_{i \in I} \lambda_i g'_i(x^*) = 0,$$

where $I := \{i : g_i(x) = 0\}$ is the index set of active constraints at x^* .

Lemma 23 *The following two statements are equivalent.*

(23.1) *The system (31) satisfies Abadie's constraint qualification.*

(23.2) *For any strictly convex quadratic function $f(x)$ on \mathbb{R}^n , x^* is the optimal solution of (34) if and only if x^* is a KKT point of (34).*

Remark. In a sense, the above lemma shows that Abadie's constraint qualification is the weakest CQ to guarantee that KKT conditions hold for optimal solutions.

Finally we show that a commonly used Slater-type constraint qualification implies Abadie's constraint qualification.

Lemma 24 [31, Theorem 28.2] *Suppose that there exists a point x^* such that $g_i(x^*) \leq 0$ for $i = 1, \dots, m$ and $g_i(x^*) < 0$ if $g_i(x)$ is not a linear function of x . Then x^* is the optimal solution of (34) if and only if x^* is a KKT point of (34).*

Lemma 25 *Suppose that there exists a point x^* such that $g_i(x^*) \leq 0$ for $i = 1, \dots, m$ and $g_i(x^*) < 0$ if $g_i(x)$ is not a linear polynomial of x . Then (31) satisfies Abadie's constraint qualification.*

4.3 Metric Regularity and Abadie's Constraint Qualification

It is well-known that metric regularity is related to Slater condition and MFCQ [28, 29, 30]. In this subsection we prove that Abadie's CQ is equivalent to metric regularity for a convex differentiable inequality system.

Definition 26 *We say that the system (31) is metrically regular at a point $\bar{x} \in S$ if there exist positive constants γ and δ such that*

$$\text{dist}(x, S) \leq \gamma \cdot \sum_{i=1}^m (g_i(x))_+ \quad \text{when } \|x - \bar{x}\| \leq \delta.$$

We say that the system (31) is metrically regular if it is metrically regular at every point in S .

Note that we are interested in metric regularity of (31) at every point in S . In general, one needs Slater condition to ensure such a metric regularity, as shown in the following lemma first proved by Robinson [28].

Lemma 27 *If there exists $x^* \in \mathbb{R}^n$ such that $g_i(x^*) < 0$ for $i = 1, \dots, m$, then (31) is metrically regular.*

Metric regularity is closely related to error bounds. In fact, metric regularity of (31) is equivalent to error bounds for infeasible solutions of (31) on bounded subset of \mathbb{R}^n .

Lemma 28 *The system (31) is metrically regular if and only if, for any number $r > 0$, there exists a positive constant $\gamma(r)$ such that*

$$\text{dist}(x, S) \leq \gamma(r) \cdot \sum_{i=1}^m (g_i(x))_+ \quad \text{when } \|x\| \leq r.$$

Now we state the main theorem in this subsection.

Theorem 29 *The system (31) is metrically regular if and only if (31) satisfies Abadie's constraint qualification.*

4.4 Error Bounds

We want to apply the main theorem in the previous subsection (Theorem 29) to a special case: (31) with convex linear/quadratic functions $g_i(x)$. In this case, the metric regularity is equivalent to the existence of a global error bound for infeasible solutions of (31). As a consequence, we obtain that Abadie's constraint qualification is a necessary and sufficient condition for a global error bound given in (32). Our result complements the study done by Luo and Luo [18], Pang and Wang [32] on error bounds for convex quadratic inequalities.

Consider the following system of convex quadratic inequalities:

$$g_i(x) \leq 0 \quad \text{for } i = 1, \dots, m, \quad (35)$$

where $g_i(x)$ are either linear or convex quadratic functions on \mathbb{R}^n .

The essence of our proof is to reduce the problem to the case that Slater condition holds. Then we can use the following result by Luo and Luo [18] to get (32).

Lemma 30 *If the system (35) satisfies the Slater condition, then there exists a positive constant γ such that*

$$\left\| \sum_{i \in I(x)} \lambda_i g'_i(x) \right\| \geq \gamma \sum_{i \in I(x)} \lambda_i \quad \text{for } x \in \mathbb{R}^n, \lambda_i \geq 0, \quad (36)$$

where $I(x) := \{i : g_i(x) = 0\}$.

It is obvious that (32) implies metric regularity. Therefore, the main effort in proving the equivalence of (32) and metric regularity is to show that metric regularity implies (32) for convex quadratic inequalities.

Theorem 31 *The convex quadratic inequality system (35) satisfies Abadie's constraint qualification if and only if there exists a positive constant γ such that*

$$\text{dist}(x, S) \leq \gamma \sum_{i=1}^m (g_i(x))_+ \quad \text{for } x \in \mathbb{R}^n, \quad (37)$$

where $S := \{x \in \mathbb{R}^n : g_i(x) \leq 0 \text{ for } i = 1, \dots, m\}$.

Note that Luo and Luo [18] proved a special case of Theorem 31: (36) holds if there exists a vector x^* such that $g(x^*) \leq 0$ and $g_i(x^*) < 0$ whenever $g_i(x)$ is not a linear function.

Theorem 31 not only gives a characterization of the existence of global error bound (32) for convex quadratic inequalities, but also reveals why there exist weak sharp minima for convex quadratic programming problems [7], as shown in the following theorem.

Theorem 32 *Assume that $f(x)$ is a convex quadratic function bounded below on $\{x \in \mathbb{R}^n : Ax \leq b\}$. Let $f_{\min} := \min_{Ax \leq b} f(x)$ and $S := \{x \in \mathbb{R}^n : Ax \leq b, f(x) = f_{\min}\}$. Then the following statements are equivalent.*

(32.1) *Abadie's constraint qualification is satisfied at every feasible point of the following inequality system:*

$$f(x) - f_{\min} \leq 0 \text{ and } Ax - b \leq 0. \quad (38)$$

(32.2) *The convex quadratic programming problem $\min_{Ax \leq b} f(x)$ has weak sharp minima. That is, there exists a positive constant γ such that*

$$f(x) \geq f_{\min} + \gamma \cdot \text{dist}(x, S) \text{ when } Ax \leq b. \quad (39)$$

(32.3) *There exists a positive constant λ such that*

$$\text{dist}(x, S) \leq \lambda ((f(x) - f_{\min})_+ + \|(Ax - b)_+\|) \text{ for } x \in \mathbb{R}^n. \quad (40)$$

Note that various characterizations of weak sharp minima of a convex quadratic programming problem were given by Ferris and Mangasarian [7]. Theorem 31 leads us to two new characterizations (32.1) and (32.3) in Theorem 32. Weak sharp minimum inequality (39) estimates how far away a feasible solution is from the solution set. The inequality (40) actually provides an estimate of the distance from any approximate solution of the quadratic programming problem to its solution set, which is more desirable when infeasible approximate solutions are involved. Even though (40) fails to be true if (38) does not satisfy Abadie's constraint qualification, one could still have the following inequality [15]:

$$\text{dist}(x, S) \leq \gamma \left(f(x) - f_{\min} + \sqrt{f(x) - f_{\min}} \right) \text{ for } Ax - b \leq 0.$$

4.5 Conclusion

We have shown that the concepts of metric regularity, error bounds, and weak sharp minimum are closely related. The essence of these concepts is to estimate the distance from an approximate solution to the solution set of the underlying problem, locally or globally. For metric regularity of parametric systems, MFCQ was proven to be a necessary and sufficient condition [29, 30]. However, for the non-parametric version of metric regularity defined here, Abadie's constraint qualification is a necessary and sufficient condition. As applications, we show that Abadie's constraint qualification is a characterization for the existence of a global error bound (32) for convex quadratic inequalities, which leads to a global error bound (40) for approximate solutions of a convex quadratic programming problem with weak sharp minima.

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5 Merit Functions for Complementarity Problems

We introduce a new merit function $P_\alpha(x)$ for a symmetric linear complementarity problem (symmetric LCP). The merit function $P_\alpha(x)$ is derived from Hestenes-Powell-Rockafellar's quadratic augmented Lagrangian function for a quadratic programming problem with simple bound constraints. The stationary points of $P_\alpha(x)$ are the solutions of the original LCP. We study various properties of $P_\alpha(x)$, including existence of global minimizers, error bounds, boundedness of level sets, and convexity of $P_\alpha(x)$. A relation between $P_\alpha(x)$ and Mangasarian and Solodov's implicit Lagrangian $M_\alpha(x)$ [27] is established. As a consequence, we recover Peng's result [30] about strict convexity of $M_\alpha(x)$ for large α and strongly monotone LCP. A Newton-type method is proposed to compute a solution of the original LCP by finding a stationary point of $P_\alpha(x)$. If $P_\alpha(x)$ is bounded below and the matrix in LCP is symmetric and nondegenerate, then the algorithm finds a solution of LCP in finitely many iterations. We also discuss possible extension to symmetric nonlinear complementarity problem. This is a summary of a paper written by the principle investigator [17].

5.1 Review on Merit Functions

Consider the following quadratic program with simple bound constraints:

$$\min_{l \leq x \leq u} \frac{1}{2} x^T Q x + q^T x, \quad (41)$$

where Q is an $n \times n$ symmetric matrix, $q \in \mathbb{R}^n$ (a vector of n components), and l, u are vectors of n components with $l \leq u$. Some components of l or u may be $-\infty$ or $+\infty$. The corresponding augmented Lagrangian function $L(x, y, \alpha)$ introduced independently by Hestenes [10, 11] and Powell [32] for equality constraints and by Rockafellar [33, 34] for inequality constraints can be written in the following unified way [15]:

$$\begin{aligned} L(x, y, \alpha) = & \frac{1}{2} x^T Q x + q^T x + \frac{\alpha}{2} \left\| \left(\frac{1}{\alpha} (x - u) - y \right)_+ \right\|^2 \\ & + \frac{\alpha}{2} \left\| \left(\frac{1}{\alpha} (l - x) + y \right)_+ \right\|^2 - \frac{\alpha}{2} \|y\|^2, \end{aligned} \quad (42)$$

where y is the Lagrangian multiplier corresponding to two-sided inequality constraints and α is a penalty parameter. Note that the Lagrangian multiplier y in (42) should satisfy the following equation:

$$y = -(Qx + q). \quad (43)$$

By substituting (43) into (42), we get a piecewise quadratic penalty function of (41) [15]:

$$L(x, -(q + Qx), \alpha) = \left(\frac{1}{2} x^T Q x + q^T x \right) - \frac{\alpha}{2} \| (Qx + q) \|^2 \\ + \frac{1}{2\alpha} \left\| \left((I - x) + \alpha(Qx + q) \right)_+ \right\|^2 + \frac{1}{2\alpha} \left\| \left((x - u) - \alpha(Qx + q) \right)_+ \right\|^2.$$

For quadratic programs with nonnegative constraints ($l_i = 0, u_i = +\infty$), we have the following penalty function:

$$P_\alpha(x) = \left(\frac{1}{2} x^T Q x + q^T x \right) - \frac{\alpha}{2} \| (Qx + q) \|^2 + \frac{1}{2\alpha} \left\| \left(\alpha(Qx + q) - x \right)_+ \right\|^2,$$

where z_+ is the vector whose i^{th} component is $\max\{0, z_i\}$. An equivalent form of $P_\alpha(x)$ was first introduced by Li and Swetits [18, 15].

In this section, we show that the augmented Lagrangian $P_\alpha(x)$ can be used as a merit function for the symmetric linear complementarity problem:

$$x \geq 0, (Qx + q) \geq 0, x^T(Qx + q) = 0. \quad (44)$$

Let the penalty parameter α be such that $0 < \alpha \|Q\| < 1$. Then x^* is a stationary point of $P_\alpha(x)$ if and only if x^* is a solution of LCP (44). Moreover, we give characterizations for the existence of a global minimizer of $P_\alpha(x)$, boundedness of level sets of $P_\alpha(x)$, and the convexity of $P_\alpha(x)$. We also derive local/global error bounds in terms of $P_\alpha(x)$.

One very interesting property of $P_\alpha(x)$ is its connection with Mangasarian and Solodov's implicit Lagrangian: $M_\alpha(x) = P_{\frac{1}{\alpha}}(x) - P_\alpha(x)$ for LCP. Based on convexity analysis of $P_\alpha(x)$, we obtain that $M_\alpha(x)$ is strictly convex if α is large and Q is positive definite, recovering a result by Peng [30].

Since $P_\alpha(x)$ is a differentiable piecewise quadratic function and its gradient $\nabla P_\alpha(x) = \frac{1}{\alpha}(I - \alpha Q)(x - (x - \alpha(Qx + q))_+)$ has a simple structure, it is very easy to design an iterative method that finds a stationary point of $P_\alpha(x)$ (or a solution of (44)) in finitely many iterations. Such an algorithm is very interesting, since almost all algorithms for quadratic programs and linear complementarity problems can be classified as either iterative or finite methods [29, 20, 1]. The most interesting property of $P_\alpha(x)$ is that, for any x^k , the Newton method starting at x^k produces an iterate x^{k+1} that is the approximate solution of (44) by using the index set $J(x^k) = \{i : (x^k - \alpha(Qx^k + q))_i > 0\}$ as the working active set for constraints

$(Qx + q) \geq 0$. That is, x^{k+1} is the solution of the following system of linear equations:

$$(Qx + q)_i = 0 \text{ for } i \in J(x^k), \quad x_i = 0 \text{ for } i \notin J(x^k),$$

whenever the above system has a unique solution. Therefore, the Newton method for finding a zero of $\nabla P_\alpha(x)$ actually corresponds to a pivotal method that allows swapping of many indices of working active sets in each step. However, it requires a strategy that makes "intelligent" index swapping to identify the active index set of a solution of (44). We show that reduction of function value of $P_\alpha(x)$ can be used for this purpose. Consider the partition of \mathbb{R}^n as a union of following polyhedral sets:

$$\mathbb{R}^n = \bigcup_J W_J,$$

where

$$W_J = \{x \in \mathbb{R}^n : (x - \alpha(Qx + q))_i \geq 0 \text{ for } i \in J, \\ (x - \alpha(Qx + q))_i \leq 0 \text{ for } i \notin J\}. \quad (45)$$

Note that W_J contains a solution x^* of (44) if and only if

$$x_i^* \geq 0, (Qx^* + q)_i = 0, \text{ for } i \in J, \\ (Qx^* + q)_i \geq 0, x_i^* = 0, \text{ for } i \notin J.$$

Therefore, our objective of using $P_\alpha(x)$ for solving (44) is to find an iterate x^k such that $W_{J(x^k)}$ contains a stationary point or a local minimizer of $P_\alpha(x)$. This can be achieved by using any descent method for a local minimizer of $P_\alpha(x)$. In general, we would like to use the Newton direction as the search direction. However, due to nonconvexity of $P_\alpha(x)$ (when Q is not positive semidefinite), the Newton method with a line search might get stuck at a nonstationary point. In such a case, we switch to a gradient direction and continue the search for a region W_J that contains a solution of (44). If the linear systems for the Newton directions are nonsingular, then our method is a natural combination of a descent method and a pivotal method. Geometrically, our method makes the iterates move toward a local minimizer of $P_\alpha(x)$; and algebraically, the iterates facilitate index swapping to make the current working active sets more and more accurate. Once the current iterate lands in a region W_J containing a stationary point of $P_\alpha(x)$ (which

is guaranteed by the descending nature of our method), the Newton method finds a stationary point of $P_\alpha(x)$ (or a solution of (44)) in one step. See Subsection 5.4 for further explanation.

Recently, there are many papers on merit functions of nonlinear complementarity problems and variational inequality problems [3, 4, 5, 9, 12, 13, 22, 25, 27, 30, 31, 35, 36]. See a survey by Fukushima [8] for more references.

The section is organized as follows. Subsection 5.2 is devoted to the discussion of properties of the merit function $P_\alpha(x)$. In Subsection 5.3, we derive new error bounds for approximate solutions of (44) in terms of $P_\alpha(x)$. In Subsection 5.4, we propose a Newton-type method for finding a solution of (44) and establish its finite termination under some mild conditions. Possible extension to symmetric nonlinear complementarity problems is discussed in Subsection 5.5. Final comments and conclusions are given in Subsection 5.6.

We conclude this subsection by introducing the notations and terminology used in this section. Let I be the $n \times n$ identity matrix. For an $n \times n$ matrix Q , Q is said to be copositive if $x^T Q x \geq 0$ for all vectors $x \geq 0$, and Q is said to be strictly copositive if $x^T Q x > 0$ for all vectors $x \geq 0, x \neq 0$. For other matrix classes mentioned in this section, we refer the reader to [1]. For $x \in \mathbb{R}^n$, $\|x\| = (\sum_{i=1}^n x_i^2)^{\frac{1}{2}}$ and $\|Q\| = \sup\{\|Qx\| : x \in \mathbb{R}^n, \|x\| = 1\}$. Let x^T (or Q^T) denote the transpose of x (or Q). For an index set J , x_J denotes the vector obtained from deleting the components of x whose indices are not in J . D^J denotes the diagonal matrix whose i^{th} diagonal entry is 1 if $i \in J$ and 0 otherwise. We use $J^c = \{i : i \notin J\}$ to denote the complement of J . For index sets J_1, J_2 , $Q_{J_1 J_2}$ is the matrix obtained from deleting the rows of Q whose indices are not in J_1 and the columns of Q whose indices are not in J_2 . For a vector $x \in \mathbb{R}^n$ and a subset K of \mathbb{R}^n , the distance from x to K is defined as follows:

$$\text{dist}(x, K) = \inf\{\|x - y\| : y \in K\}.$$

If K is closed and convex, the orthogonal projection of x to K is the unique vector x^* in K such that $\|x - x^*\| = \text{dist}(x, K)$. In the case that K is a union of finitely many polyhedral sets, such as the set of local/global minimizers of $P_\alpha(x)$, there might be several x^* 's in K such that $\|x - x^*\| = \text{dist}(x, K)$. In such a case, let us assume that $\Pi_K(x)$ is a vector in K such that $\|x - \Pi_K(x)\| = \text{dist}(x, K)$. The sign of a real number t is denoted by $\text{sign}(t)$.

5.2 Properties of Merit Function $P_\alpha(x)$

Recently, there are much attention given to merit functions for the following nonlinear complementarity problem [3, 4, 5, 9, 12, 13, 22, 25, 27, 30, 31, 35, 36]:

$$x \geq 0, F(x) \geq 0, x^T F(x) = 0, \quad (46)$$

where $F(x) : \mathbb{R}^n \rightarrow \mathbb{R}^n$ is differentiable.

One standard approach of constructing a merit function for (46) is to find a function $M(x) \geq 0$ such that x^* is a solution of (46) if and only if $M(x^*) = 0$. As a result, (46) can be reformulated as an unconstrained (global) minimization of $M(x)$. (For merit functions with constraints or reformulations of (46) as a constrained minimization problem, see a survey by Fukushima [8].) Such approaches lead to Mangasarian and Solodov's implicit Lagrangian [27]:

$$M_\alpha(x) = x^T F(x) + \frac{1}{2\alpha} \left(\|(x - \alpha F(x))_+\|^2 - \|x\|^2 + \|(F(x) - \alpha x)_+\|^2 - \|F(x)\|^2 \right),$$

and Bermeister and Fischer's NCP-function [4, 5]:

$$\Psi(x) = \frac{1}{2} \sum_{i=1}^n \left(\sqrt{x_i^2 + F_i(x)^2} - x_i - F_i(x) \right)^2.$$

However, it is difficult to design an algorithm for computing a zero (or a global minimizer) of a nonnegative function $M(x)$. Most numerical methods can only find a stationary point or a local minimizer of $M(x)$, which might not be a solution of (46). Therefore, it is important to know when the stationary points of a merit function $M(x)$ are actually solutions of (46). Another issue about a merit function is whether or not its level sets are bounded. In general, it is not easy to ensure the convergence of iterates generated by a descent method for minimizing a nonconvex function. However, if a merit function $M(x)$ has bounded level sets, then a minimizing sequence for $M(x)$ is bounded and has at least one cluster point.

Unlike $M_\alpha(x)$ and $\Psi(x)$, the merit function $P_\alpha(x)$ exploits linearity of $F(x) = Qx + q$ and symmetry of Q . As a result, it preserves the structure of original LCP (44) and has many properties that $M_\alpha(x)$ and $\Psi(x)$ do not have. In this subsection, we give complete characterizations for various properties of $P_\alpha(x)$, including equivalence of stationary points of $P_\alpha(x)$ and

solutions of (44), existence of global minimizers, boundedness of level sets, and convexity of $P_\alpha(x)$. We also discuss the convexity of $M_\alpha(x)$ by using the relation $M_\alpha(x) = P_{\frac{1}{\alpha}}(x) - P_\alpha(x)$.

5.3 Stationary Points and Convexity

In general, stationary points of $M_\alpha(x)/\Psi(x)$ are not necessarily solutions of (46) and there is no known relation between the convexity of $M_\alpha(x)/\Psi(x)$ and the monotonicity of $F(x)$, even if $F(x) = Qx + q$. Recently, Peng [30] proved the strict convexity of $M_\alpha(x)$ for large α and strongly monotone LCP. In this subsection, we obtain the equivalence of stationary points of $P_\alpha(x)$ and the solutions of (44), as well as the equivalence of the convexity of $P_\alpha(x)$ and the monotonicity of (44). For a positive definite Q , we show that $P_\alpha(x)$ is strictly convex for small α and strictly concave for large α . We also establish a relation between $M_\alpha(x)$ and $P_\alpha(x)$: $M_\alpha(x) = P_{\frac{1}{\alpha}}(x) - P_\alpha(x)$. As a consequence, we recover Peng's result [30] on strict convexity of $M_\alpha(x)$.

Note that definition of $P_\alpha(x)$ does not require the symmetry of $P_\alpha(x)$. Therefore, some properties of $P_\alpha(x)$ in this subsection are given for an arbitrary $n \times n$ matrix Q .

Theorem 33 *For any $n \times n$ matrix Q ,*

$$\nabla P_\alpha(x) = \frac{1}{\alpha}(I - \alpha Q^T) \left(x - \left(x - \alpha(Qx + q) \right)_+ \right) + \frac{1}{2}(Q^T - Q)x. \quad (47)$$

If Q is symmetric, then

$$\nabla P_\alpha(x) = \frac{1}{\alpha}(I - \alpha Q) \left(x - \left(x - \alpha(Qx + q) \right)_+ \right). \quad (48)$$

Theorem 34 *Suppose that Q is symmetric and $0 < \alpha\|Q\| < 1$. Then x^* is a stationary point of $P_\alpha(x)$ if and only if x^* is a solution of (44).*

Remark. Stronger conditions are required for the equivalence of stationary points of $M_\alpha(x)/\Psi(x)$ and the solutions of (46). Yamashita and Fukushima [36] proved that x is a stationary point of $M_\alpha(x)$ ($\alpha > 1$) if and only if x solves (46), under the assumption that $\nabla F(x)$ is positive definite for every $x \in \mathbb{R}^n$. Independently, Jiang [12] proved the same result under the assumption that $\nabla F(x)$ is a P -matrix for every $x \in \mathbb{R}^n$. Yamashita and Fukushima [36] also showed that there exists a (nonlinear) strictly monotone function $F(x)$ such that some stationary point of $M_\alpha(x)$ is not a solution of

(46). For the merit function $\Psi(x)$, Geiger and Kanzow [9] proved that x is a stationary point of Ψ if and only if x solves (46), under the assumption that $\nabla F(x)$ is positive semidefinite for every $x \in \mathbb{R}^n$. Independently, Facchinei and Soares [3] proved the same result under the assumption that $F(x)$ is P_0 -function.

In the case that $F(x) = Qx + q$ and Q is symmetric, these results lead to the equivalence of stationary points of $\Psi(x)$ (or $M_\alpha(x)$) and the solutions of (46) under the assumption that Q is positive semidefinite (or Q is positive definite). However, for positive semidefinite Q , the augmented Lagrangian $P_\alpha(x)$ is actually convex.

For convexity analysis of $P_\alpha(x)$, we need the following lemma about convexity of a differentiable piecewise quadratic function.

Lemma 35 [19, Lemma 2.1] *Let $g(x)$ be a differentiable piecewise quadratic function and $\nabla g(x) = Bx + b + \beta C^T(Cx + c)_+$. If B and $(B + \beta C^T C)$ are positive semidefinite (or positive definite), then $g(x)$ is a convex (or strictly convex) function.*

Theorem 36 *Suppose that Q is symmetric and $0 < \alpha\|Q\| < 1$. Then $P_\alpha(x)$ is convex (or strictly convex) if and only if Q is positive semidefinite (or positive definite).*

For nonsymmetric Q , we can still characterize the strict convexity of $P_\alpha(x)$.

Theorem 37 *Suppose that Q is an $n \times n$ matrix. Then the following statements are equivalent.*

- 1°. Q is positive definite.
- 2°. There is $\epsilon > 0$ such that $P_\alpha(x)$ is strictly convex for $0 < \alpha < \epsilon$.
- 3°. There is $\lambda > 0$ such that $P_\alpha(x)$ is strictly concave for $\alpha > \lambda$.

Remark. The above proof also shows that $P_\alpha(x)$ is convex for small α if and only if Q is positive semidefinite and $Qx = 0$ whenever $x^T Qx = 0$. Moreover, $P_\alpha(x)$ can not be concave for large α if Q is not positive definite.

With Theorem 37, we can derive the strict convexity of $M_\alpha(x)$ for affine and strongly monotone $F(x)$ by using the following representation of $M_\alpha(x)$ by $P_\alpha(x)$.

Theorem 38 Suppose that $F(x) = Qx + q$ and $\alpha > 0$. Then, $M_\alpha(x) = P_{\frac{1}{\alpha}}(x) - P_\alpha(x)$ and $M_\alpha(x) = -M_{\frac{1}{\alpha}}(x)$.

With Theorem 37 and Theorem 38, we recover the following corollary about the strict convexity/concavity of $M_\alpha(x)$ for affine and strongly monotone $F(x)$, which was first proved by Peng [30, Theorem 3.1].

Corollary 39 Suppose that $F(x) = Qx + q$ and Q is positive definite. Then $M_\alpha(x)$ is a strictly convex function if

$$\alpha > \max \left\{ \|Q\|, \|Q^{-1}\|, 2 \left\| (Q^{-1} + (Q^{-1})^T)^{-1} \right\|, 2 \left\| (Q + Q^T)^{-1} \right\| \right\}. \quad (49)$$

Moreover, $M_\alpha(x)$ is a strictly concave function if

$$\alpha < \min \left\{ \frac{1}{\|Q\|}, \frac{1}{\|Q^{-1}\|}, \frac{1}{2 \left\| (Q^{-1} + (Q^{-1})^T)^{-1} \right\|}, \frac{1}{2 \left\| (Q + Q^T)^{-1} \right\|} \right\}. \quad (50)$$

Remark. Note that the lower bound of α for the strict convexity of $M_\alpha(x)$ given by Peng [30, Theorem 3.1] is

$$\alpha > \max_{\|x\|=1} \frac{1 + x^T Q^T Q x}{2x^T Q x}.$$

In the case that Q is symmetric, then

$$\max_{\|x\|=1} \frac{1 + x^T Q^T Q x}{2x^T Q x} \leq \frac{1}{2}(\|Q^{-1}\| + \|Q\|) \leq \max\{\|Q\|, \|Q^{-1}\|\}.$$

Thus, Peng's lower bound for α is sharper than (49).

So far, we are not aware of any result on convexity of $\Psi(x)$. Luo and Tseng [25] introduced another class of differentiable merit functions related to $\Psi(x)$ that are convex if $F(x)$ is monotone.

5.4 Global Minimizers and Bounded Level Sets

Unlike $M_\alpha(x)$ and $\Psi(x)$, which are based on the equivalence of the global minimizers of the merit function and the solutions of (46), $P_\alpha(x)$ might not have a global minimizer. This is undesirable. However, we show that $P_\alpha(x)$ is bounded below and has bounded level sets if Q is strictly copositive. We

also give characterizations for the existence of a global minimizer of $P_\alpha(x)$ and for boundedness of level sets of $P_\alpha(x)$.

The existence of global minimizers of $P_\alpha(x)$ and boundedness of level sets of $P_\alpha(x)$ are closely related to the behavior of the following quadratic programming problem:

$$\min_{x \geq 0} \frac{1}{2} x^T Q x + q^T x. \quad (51)$$

Lemma 40 [15] *Suppose that Q is symmetric and $0 < 2\|Q\| < 1$. Then the quadratic programming problem (51) has a global solution if and only if $P_\alpha(x)$ has a global minimizer. Moreover, x^* is a local (or isolated local) solution of (41) if and only if x^* is a local (or isolated local) minimizer of $P_\alpha(x)$.*

The above lemma shows that the the reformulation of (51) as unconstrained minimization of $P_\alpha(x)$ does not change any intrinsic characteristics of (51). The above lemma reduces the existence of a global minimizer of $P_\alpha(x)$ to the problem of the existence of a global solution of (51). Eaves [2] proved that the existence of a global solution of a quadratic programming problem is equivalent to the lower boundedness of the objective function on any ray in the feasible set.

Lemma 41 [2, Corollary 8] *The quadratic programming problem (51) has a global solution if and only if Q is copositive and $q^T x \geq 0$, whenever $x \geq 0$ and $x^T Q x = 0$.*

Putting all these results together, we have the following characterizations for the existence of a global minimizer of $P_\alpha(x)$.

Theorem 42 *Suppose that Q is symmetric and $0 < 2\alpha\|Q\| < 1$. Then the following statements are equivalent:*

- 1°. $P_\alpha(x)$ has a global minimizer.
- 2°. $P_\alpha(x)$ is bounded below.
- 3°. The quadratic program (51) has a global solution.
- 4°. Q is copositive and $q^T x \geq 0$, whenever $x \geq 0$ and $x^T Q x = 0$.

In order to give a characterization for boundedness of level sets of $P_\alpha(x)$, we need the following two lemmas about the connection between $P_\alpha(x)$ and the objective function of (51).

Lemma 43 [15] Suppose that $\alpha > 0$. Then $P_\alpha(x) \leq \frac{1}{2}x^T Qx + q^T x$ if $x \geq 0$.

Lemma 44 Let $f(x) = \frac{1}{2}x^T Qx + q^T x$, $E = (I - \alpha Q)$, and $x^0 = \alpha E^{-1}q$. Then, for any index set J and $x \in W_J$,

$$P_\alpha(x) \geq P_\alpha(x^0) + g_J \left(D^{J^c}(x - x^0), D^J Q D^J (x - x^0) \right) + f \left(D^J (Ex - \alpha q) \right),$$

where W_J is defined as in (45), $g_J(y, z)$ is a strictly convex quadratic function of (y, z) , $J^c = \{i : i \notin J\}$, and D^J denotes the diagonal matrix whose i^{th} diagonal entry is 1 if $i \in J$ and 0 otherwise.

In the following theorem, we give two characterizations for boundedness of level sets of $P_\alpha(x)$: one in terms of boundedness of level sets for (51) and another in terms of Q and q .

Theorem 45 Suppose that Q is symmetric and $0 < 2\alpha\|Q\| < 1$. Then the following statements are equivalent:

- 1°. $P_\alpha(x)$ has bounded level sets.
- 2°. The level set for (51), $\{x \in \mathbb{R}^n : x \geq 0, \frac{1}{2}x^T Qx + q^T x \leq \gamma\}$, is bounded for every $\gamma < \infty$.
- 3°. Q is copositive and $q^T x > 0$, whenever $x \geq 0$, $x \neq 0$, and $x^T Qx = 0$.

Corollary 46 Suppose that Q is symmetric and strictly copositive. Then the level sets of $P_\alpha(x)$ are bounded if $0 < 2\alpha\|Q\| < 1$.

Remark. Yamashita and Fukushima [36] proved that $M_\alpha(x)$ ($\alpha > 1$) has bounded level sets if $F(x)$ is strongly monotone and Lipschitz continuous. For merit function $\Psi(x)$, Geiger and Kanzow [9] proved that the level sets of Ψ are bounded if $F(x)$ is strongly monotone. Independently, Facchinei and Soares [3] proved that the level sets of Ψ are bounded if $F(x)$ is a uniformly P -function.

5.5 Local and Global Error Bounds

Let S^* be the solutions of (44), L^* be the set of local minimizers of $P_\alpha(x)$, and G^* be the set of global minimizers of $P_\alpha(x)$. Then, for $0 < \alpha\|Q\| < 1$, we have $G^* \subset L^* \subset S^*$. In general, $G^* \neq L^*$, $L^* \neq S^*$, and $G^* \neq S^*$. However, if Q is positive semidefinite, then $P_\alpha(x)$ is convex for $0 < \alpha\|Q\| < 1$ (cf.

Theorem 36) and $G^* = L^* = S^*$. There are many results about error estimates for $\text{dist}(x, S^*)$, the distance from x to S^* . See [23, 24, 28, 26, 14, 22, 21] and references therein. For $0 < \alpha\|Q\| < 1$, $(I - \alpha Q)$ is a positive definite matrix and, by Theorem 33, we have $\|\nabla P_\alpha(x)\| \approx \|x - (x - \alpha(Qx + q))_+\|$. Thus, known error bounds in terms of $\|x - (x - \alpha(Qx + q))_+\|$ can be rewritten in terms of $\|\nabla P_\alpha(x)\|$. In this subsection, we derive local/global error estimates of $\text{dist}(x, L^*)$ and $\text{dist}(x, G^*)$ in terms of $P_\alpha(x)$.

5.6 Local Error Bounds

Since $P_\alpha(x)$ can not distinguish stationary points of $P_\alpha(x)$ from nonstationary points of $P_\alpha(x)$, we can not use expressions of $P_\alpha(x)$ to estimate $\text{dist}(x, S^*)$. However, we can use $P_\alpha(x)$ to estimate the distance from x to the set of local/global minimizers of $P_\alpha(x)$.

First we need the following lemma about the structure of L^* and G^* .

Lemma 47 *Suppose that Q is symmetric, $\alpha > 0$, and $W \cap S^*$ is a polyhedral set. Then $W \cap S^* = W \cap L^*$ if $W \cap L^* \neq \emptyset$ and $W \cap S^* = W \cap G^*$ if $W \cap G^* \neq \emptyset$.*

The next lemma gives error bounds on each polyhedral set W_J .

Lemma 48 *Suppose that Q is symmetric and $0 < 2\alpha\|Q\| < 1$. Then there exists a positive constant γ such that*

$$\frac{1}{\gamma} \sqrt{P_\alpha(x) - P_\alpha(\Pi_{W_J \cap L^*}(x))} \leq \text{dist}(x, W_J \cap L^*) \leq \gamma \sqrt{P_\alpha(x) - P_\alpha(\Pi_{W_J \cap L^*}(x))}$$

for $x \in W_J$ with $W_J \cap L^* \neq \emptyset$.

In order to replace $\text{dist}(x, W_J \cap L^*)$ by $\text{dist}(x, L^*)$, we need the following lemma for lower bound of $\text{dist}(x, L^*)$ or $\text{dist}(x, G^*)$.

Lemma 49 *There exists a positive constant ϵ such that*

$$\|x - x^*\| \geq \epsilon \sqrt{|P_\alpha(x) - P_\alpha(x^*)|} \quad \text{for } x \in \mathbb{R}^n, x^* \in S^*. \quad (52)$$

Theorem 50 *Suppose that Q is symmetric and $0 < 2\alpha\|Q\| < 1$. Let L^* be the (nonempty) set of local minimizers of $P_\alpha(x)$. Then there exist positive constants δ, η such that, for $x \in \mathbb{R}^n$ with $\text{dist}(x, L^*) \leq \delta$,*

$$\frac{1}{\eta} \sqrt{P_\alpha(x) - P_\alpha(\Pi_{L^*}(x))} \leq \text{dist}(x, L^*) \leq \eta \sqrt{P_\alpha(x) - P_\alpha(\Pi_{L^*}(x))}. \quad (53)$$

Theorem 51 Suppose that Q is symmetric and $0 < 2\alpha\|Q\| < 1$. Let G^* be the (nonempty) set of global minimizers of $P_\alpha(x)$. Then there exist positive constants δ, η such that, for $x \in \mathbb{R}^n$ with $\text{dist}(x, G^*) \leq \delta$,

$$\frac{1}{\eta} \sqrt{P_\alpha(x) - P_{\alpha, \min}} \leq \text{dist}(x, G^*) \leq \eta \sqrt{P_\alpha(x) - P_{\alpha, \min}}, \quad (54)$$

where $P_{\alpha, \min} = \inf\{P_\alpha(x) : x \in \mathbb{R}^n\}$.

5.7 Global Error Bounds

In general, (53) and (54) do not hold if x is an arbitrary vector in \mathbb{R}^n . In this subsection, we give characterizations for the existence of global error bounds for $\text{dist}(x, G^*)$. Note that we can not use $\sqrt{P_\alpha(x) - P_\alpha(\Pi_{L^*}(x))}$ as a global measure of $\text{dist}(x, L^*)$, since it is likely to have some $x \in \mathbb{R}^n \setminus L^*$ such that $P_\alpha(x) = P_\alpha(\Pi_{L^*}(x))$.

Theorem 52 Suppose that Q is symmetric and $0 < 2\alpha\|Q\| < 1$. Then the following statements are equivalent.

- 1°. $P_\alpha(x)$ is bounded below for every $q \in \mathbb{R}^n$.
- 2°. $P_\alpha(x)$ has bounded level sets for every $q \in \mathbb{R}^n$.
- 3°. Q is strictly copositive.
- 4°. For any q , $P_{\alpha, \min} = \inf\{P_\alpha(x) : x \in \mathbb{R}^n\} > -\infty$ and there exists a positive constant $\gamma = \gamma(Q, q)$ such that

$$\frac{1}{\gamma} \sqrt{P_\alpha(x) - P_{\alpha, \min}} \leq \text{dist}(x, G^*) \leq \gamma \sqrt{P_\alpha(x) - P_{\alpha, \min}} \quad \text{for } x \in \mathbb{R}^n.$$

Note that $G^* \subset L^* \subset S^*$. In general, $G^* \neq L^*$, $L^* \neq S^*$, and $G^* \neq S^*$. However, if Q is positive semidefinite, then $P_\alpha(x)$ is convex for $0 < \alpha\|Q\| < 1$ (cf. Theorem 36) and $G^* = L^* = S^*$. In this case, we have the following global error bound for symmetric and monotone linear complementarity problems (cf. Corollary 2.8 in [14]).

Theorem 53 Suppose that Q is symmetric and positive semidefinite, $0 < \alpha\|Q\| < 1$, and the solution set S^* of (44) is not empty. Then there exists a positive constant γ such that

$$\text{dist}(x, S^*) \leq \gamma \left((P_\alpha(x) - P_{\alpha, \min}) + \sqrt{P_\alpha(x) - P_{\alpha, \min}} \right) \quad \text{for } x \in \mathbb{R}^n.$$

5.8 A Newton-Type Method

By exploiting the structure of $\nabla P_\alpha(x)$, we can get an iterative algorithm for finding a solution of (44) in finitely many iterations.

Algorithm 54 Suppose that Q is symmetric and the principle submatrices of Q are nonsingular (i.e., Q is nondegenerate). Then generate a sequence of iterates as follows:

Step 0. choose positive constants $\delta > 0$, $0 < \beta \leq \gamma < 1$, $0 < 2\alpha\|Q\| < 1$;
set $b = -\alpha q$ and $E = (I - \alpha Q)$; let $k = 0$ and $x^0 \in \mathbb{R}^n$;

Step 1. compute $r^k = x^k - (Ex^k + b)_+$;

Step 2. if $r^k = 0$, then output the solution x^k and stop;

Step 3. let $J_k = \{i : (Ex^k + b)_i > 0\}$ and $\bar{J}_k = \{i : (Ex^k + b)_i \leq 0\}$;

Step 4. let $u_{J_k}^k = Q_{J_k J_k}^{-1} \left(Q_{J_k \bar{J}_k} r_{\bar{J}_k}^k - \frac{1}{\alpha} r_{J_k}^k \right)$ and $u_{\bar{J}_k}^k = -r_{\bar{J}_k}^k$;

Step 5. if $x^k + u^k = (E(x^k + u^k) + b)_+$, then output the solution x^k and stop;

Step 6. if $|(r^k)^T u^k| \geq \delta \|r^k\|^2$, $z^k = u^k$; else, $z^k = -r^k$;

Step 7. let $\beta \leq \eta_k \leq \gamma$ and find the stepsize $t_k \neq 0$ such that

$$-\text{sign}(t_k)(z^k)^T \nabla P_\alpha(x^k + t_k z^k) = \eta_k |(z^k)^T \nabla P_\alpha(x^k)| \quad (55)$$

and, for t between 0 and t_k ,

$$-\text{sign}(t_k)(z^k)^T \nabla P_\alpha(x^k + t z^k) \geq \eta_k |(z^k)^T \nabla P_\alpha(x^k)|; \quad (56)$$

Step 8. set $x^{k+1} = x^k + t_k z^k$;

Step 9. update k by $k + 1$ and go back to Step 1.

Remark. The algorithm is very much like a Newton method for solving the piecewise linear equation: $x - (x - \alpha(Qx + q))_+ = 0$. Note that the Newton direction u^k for $P_\alpha(x)$ at x^k is the solution of the following linear system:

$$\frac{1}{\alpha}(I - \alpha Q)(I - D^{J_k}(I - \alpha Q))u = -\nabla P_\alpha(x^k) = -\frac{1}{\alpha}(I - \alpha Q)r^k,$$

or equivalently,

$$(I - D^{J_k}(I - \alpha Q))u = -r^k. \quad (57)$$

That is, the Newton direction for $P_\alpha(x)$ is the Newton direction for the equation: $x - (x - \alpha(Qx + q))_+ = 0$.

We can rewrite (57) as follows:

$$u_i = -r_i^k \quad \text{for } i \notin J_k, \quad \alpha(Qu)_i = -r_i^k \quad \text{for } i \in J_k. \quad (58)$$

Using matrix and vector partition, we can write the second set of equations in (58) as

$$\alpha Q_{J_k J_k} u_{J_k} + \alpha Q_{J_k \bar{J}_k} u_{\bar{J}_k} = -r_{J_k}^k. \quad (59)$$

Thus, by (58) and (59), we get that $u_{\bar{J}_k}^k = -r_{\bar{J}_k}^k$ and

$$u_{J_k}^k = Q_{J_k J_k}^{-1} \left(Q_{J_k \bar{J}_k} r_{\bar{J}_k}^k - \frac{1}{\alpha} r_{J_k}^k \right).$$

Therefore, it is possible to use matrix updating techniques for computing the inverse of $Q_{J_k J_k}$. If Q is a sparse matrix, then (58) is also a sparse linear system. If $Q_{J_k J_k}$ is nonsingular and W_{J_k} contains a stationary point of $P_\alpha(x)$, then $(x^k + u^k)$ is the stationary point of the quadratic function $P_\alpha(x)$ on W_{J_k} .

The line search can be done in at most $\mathcal{O}(n^2)$ operations. Note that

$$h(t) = \alpha(z^k)^T \nabla P_\alpha(x^k + tz^k) = a_0 + a_1 t - \sum_{i=1}^n c_i (c_i t - d_i)_+,$$

where $a_0 = (z^k)^T E x^k$, $a_1 = (z^k)^T E z^k$, $d_i = -(E x^k + b)_i$, and $c_i = (E z^k)_i$. Without loss of generality, we assume that $c_i \neq 0$. (If $c_i = 0$, delete $c_i(c_i t + d_i)_+$ from the summation.) Let $y_i = \frac{d_i}{c_i}$. After a sorting of $\{y_1, \dots, y_n\}$ and relabeling (with $\mathcal{O}(n \log n)$ operations), we may assume

$$y_1 \leq y_2 \leq \dots \leq y_n.$$

If $h(0) < 0$, we can evaluate $h(y_i)$ for $y_i > 0$ and find $y_r > 0$ such that $h(y_r) \geq \eta_k h(0)$ and $h(y_i) < \eta_k h(0)$ for $0 < y_i < y_r$. If $y_{r-1} \geq 0$, let $\bar{y}_{r-1} = y_{r-1}$; else, $\bar{y}_{r-1} = 0$. Then there exists a unique $t_k \in [\bar{y}_{r-1}, y_r]$ that can be used as our stepsize. Note that t_k is the unique solution of the following linear equation:

$$a_0 + a_1 t - \sum_{c_i > 0, y_i \geq \bar{y}_{r-1}} c_i (c_i t - d_i) - \sum_{c_i < 0, y_i \leq y_{r-1}} c_i (c_i t - d_i) = \eta_k h(0).$$

Similarly, if $h(0) > 0$, then we can find a stepsize $t_k < 0$ such that (55) and (56) hold.

We can use any descent method for minimization of $P_\alpha(x)$ to identify an active index set of a solution of (44). The above algorithm tries to take advantage of the Newton directions in minimization process.

Now we state the finite termination of Algorithm 54.

Theorem 55 *Suppose that Q is symmetric, the principle submatrices of Q are nonsingular, and (51) is bounded below. Then, for any given initial guess x^0 and $0 < \beta \leq \gamma < 1$, Algorithm 54 always finds a solution of (44) in finitely many iterations.*

Remark. The assumption that principle submatrices of Q is nonsingular is not essential. It is possible not to use this assumption in the design of an iterative algorithm that terminates in finite iterations (cf. [18]).

5.9 Extension

Consider the nonlinear complementarity problem (46). Assume that $F(x)$ is a conservative field or $\nabla F(x)$ is symmetric; i.e.,

$$\frac{\partial F_j}{\partial x_i} = \frac{\partial F_i}{\partial x_j}, \quad \text{for } 1 \leq i, j \leq n.$$

Then there exists a potential function $f(x)$ of $F(x)$ such that

$$\frac{\partial f}{\partial x_i} = F_i, \quad \text{for } 1 \leq i \leq n.$$

We use the following notation to denote such a potential function:

$$f(x) = \int_0^x F(y) dy \equiv \sum_{i=1}^n \int_C F_i(y) dy_i,$$

where the integration is the line integral in differential form and C is any smooth curve starting at 0 and ending at x . Using the potential function $f(x)$ of $F(x)$, we can define the following merit function for (46):

$$P_\alpha(x) = \int_0^x F(y) dy - \frac{\alpha}{2} \|F(x)\|^2 + \frac{1}{2\alpha} \left\| (\alpha F(x) - x)_+ \right\|^2.$$

Note that

$$\nabla P_\alpha(x) = \frac{1}{\alpha} (I - \alpha \nabla F(x)) \left(x - (x - \alpha F(x))_+ \right).$$

Therefore, if $0 < \alpha \|\nabla F(x)\| < 1$ for $x \in \mathbb{R}^n$, then the stationary points of $P_\alpha(x)$ are the solutions of the symmetric nonlinear complementarity problem (46).

However, if $\nabla F(x)$ is not bounded, then we can not use a fixed α for all x . One possible remedy is to adjust the values dynamically. That is, we choose α_k such that $0 < \alpha_k \|\nabla F(x^k)\| < 1$ and generate x^{k+1} by minimizing $P_{\alpha_k}(x)$ with starting point x^k .

5.10 Conclusions

We have studied many properties of the augmented Lagrangian $P_\alpha(x)$ for symmetric linear complementarity problems. Unlike merit functions $M_\alpha(x)$ and $\Psi(x)$, stationary points of $P_\alpha(x)$ are always solutions of (44) if $0 < \alpha \|Q\| < 1$. Also the merit function $P_\alpha(x)$ is convex if the original LCP (44) is monotone. However, $P_\alpha(x)$ is not always bounded below. We have derived characterizations for the existence of global minimizers and the boundedness of level sets of $P_\alpha(x)$. In particular, if Q is strictly copositive, then $P_\alpha(x)$ has bounded level sets.

One interesting result is the connection between $P_\alpha(x)$ and Mangasarian and Solodov's implicit Lagrangian $M_\alpha(x)$: $M_\alpha(x) = P_{\frac{1}{\alpha}}(x) - P_\alpha(x)$. Based on the convexity analysis of $P_\alpha(x)$, we have recovered a result by Peng [30] about strict convexity of $M_\alpha(x)$ for large α and strongly monotone LCP. Since $M_\alpha(x) = -M_{\frac{1}{\alpha}}(x)$, $M_\alpha(x)$ is a strictly concave function for small α , if $F(x) = Qx + q$ and Q is positive definite. This sheds new light on the fact that Mangasarian and Solodov [27] reformulate (46) as unconstrained (global) minimization of $M_\alpha(x)$ for $\alpha > 1$ and Tseng, Yamashita, and Fukushima [35] reformulate (46) as unconstrained (global) maximization of $M_\alpha(x)$ for $0 < \alpha < 1$.

A convenient choice of α is by using the supremum norm of Q :

$$\bar{\alpha} = \frac{1}{3 \max_{1 \leq i \leq n} \sum_{j=1}^n |Q_{ij}|}. \quad (60)$$

Then $0 < 2\bar{\alpha}\|Q\| < 1$. Let

$$P_{Q,q}(x) = \left(\frac{1}{2}x^T Qx + q^T x \right) - \frac{\bar{\alpha}}{2}\|(Qx + q)\|^2 + \frac{1}{2\bar{\alpha}}\left\| \left(\bar{\alpha}(Qx + q) - x \right)_+ \right\|^2.$$

Then it is very easy to verify that $P_{\theta Q, \theta q}(x) = P_{Q,q}(x)$ for $\theta > 0$. That is, the augmented Lagrangian $P_{Q,q}(x)$ is invariant with respect to the scaling of (44). Since the scaling of (44) does not change the characteristics of (44), it is natural to require that merit functions for (46) keep the intrinsic characteristics of (46) and be invariant with respect to scaling of the original complementarity problem, as pointed out by J. Moré during his talk at the International Conference on Complementarity Problems.

Even though $P_\alpha(x)$ has many desirable properties, it requires the symmetry of $\nabla F(x)$ and linearity of $F(x)$. For nonlinear $F(x)$ with symmetric Jacobian $\nabla F(x)$, $P_\alpha(x)$ can be defined by using a potential function of $F(x)$ and the stationary points of $P_\alpha(x)$ are solutions of (46) if $\|\nabla F(x)\|$ is bounded and α is small enough. Further study is necessary to understand the behavior of $P_\alpha(x)$ for symmetric nonlinear complementarity problems.

Since $M_\alpha(x)$ is also a differentiable piecewise quadratic function, it is possible to use a Newton-type method for finding a stationary point of $M_\alpha(x)$ in finitely many steps. However, the equations for Newton directions of $M_\alpha(x)$ are not as easy to solve as those for Newton directions of $P_\alpha(x)$.

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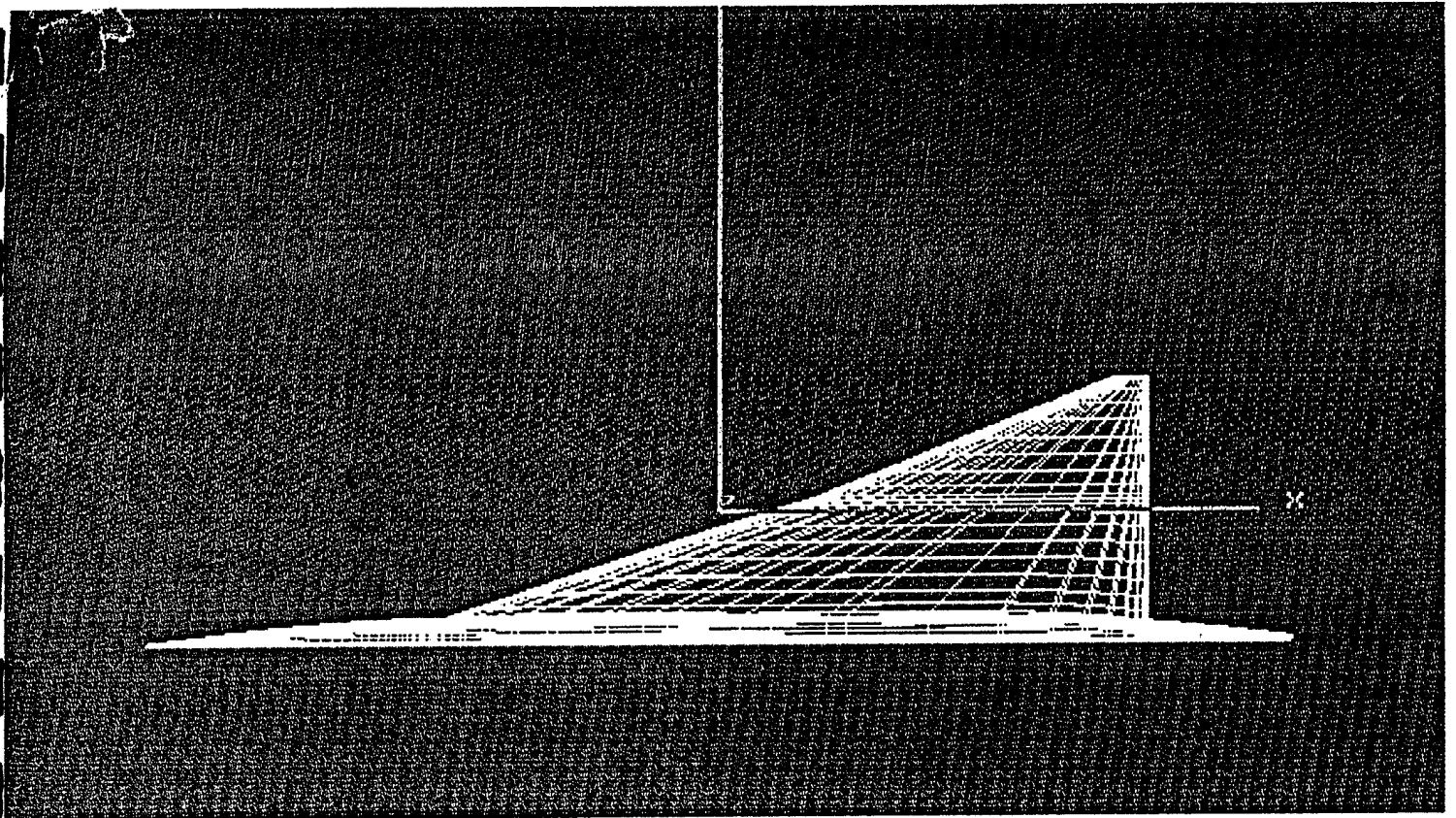


Figure 1: Actual Data

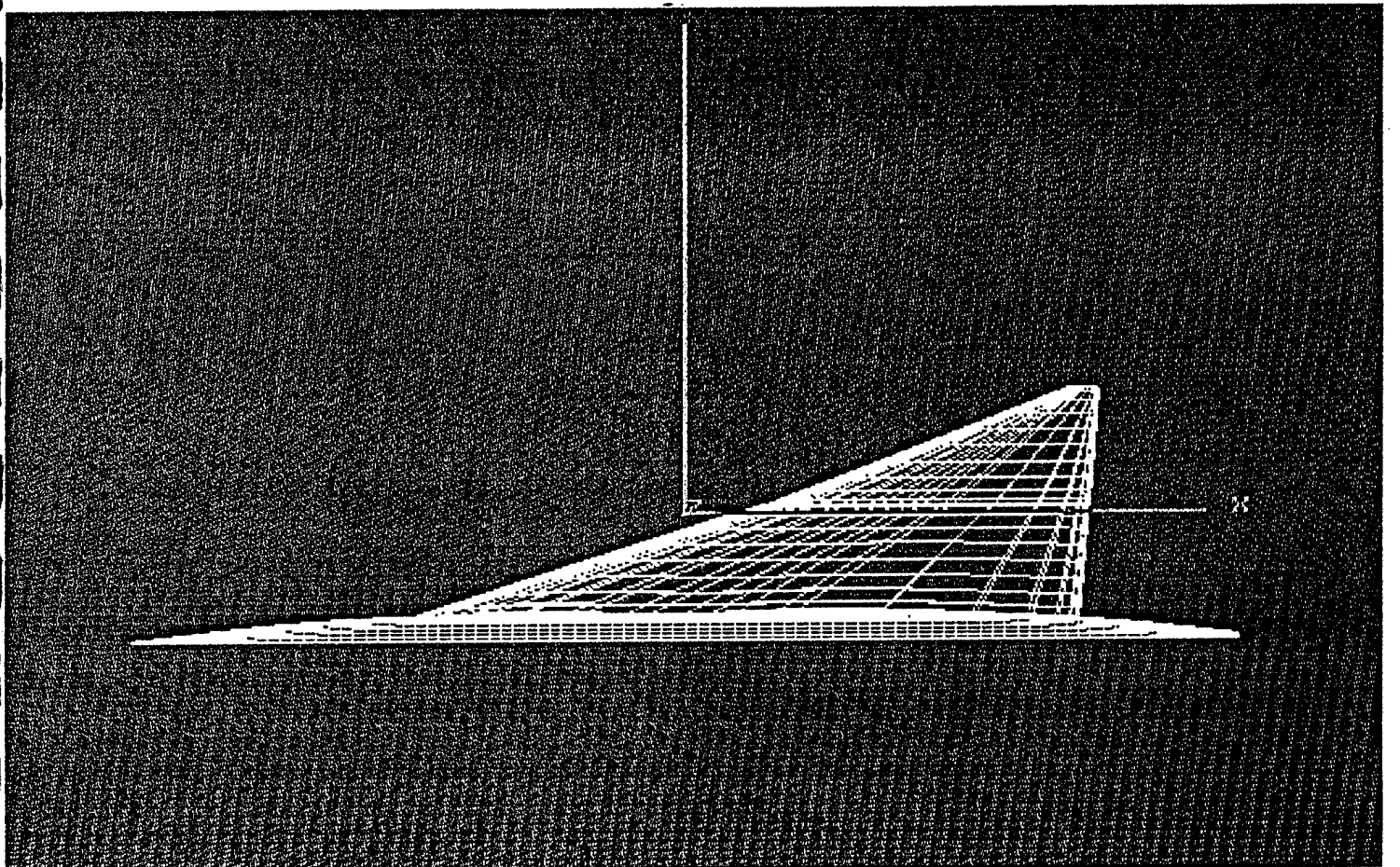
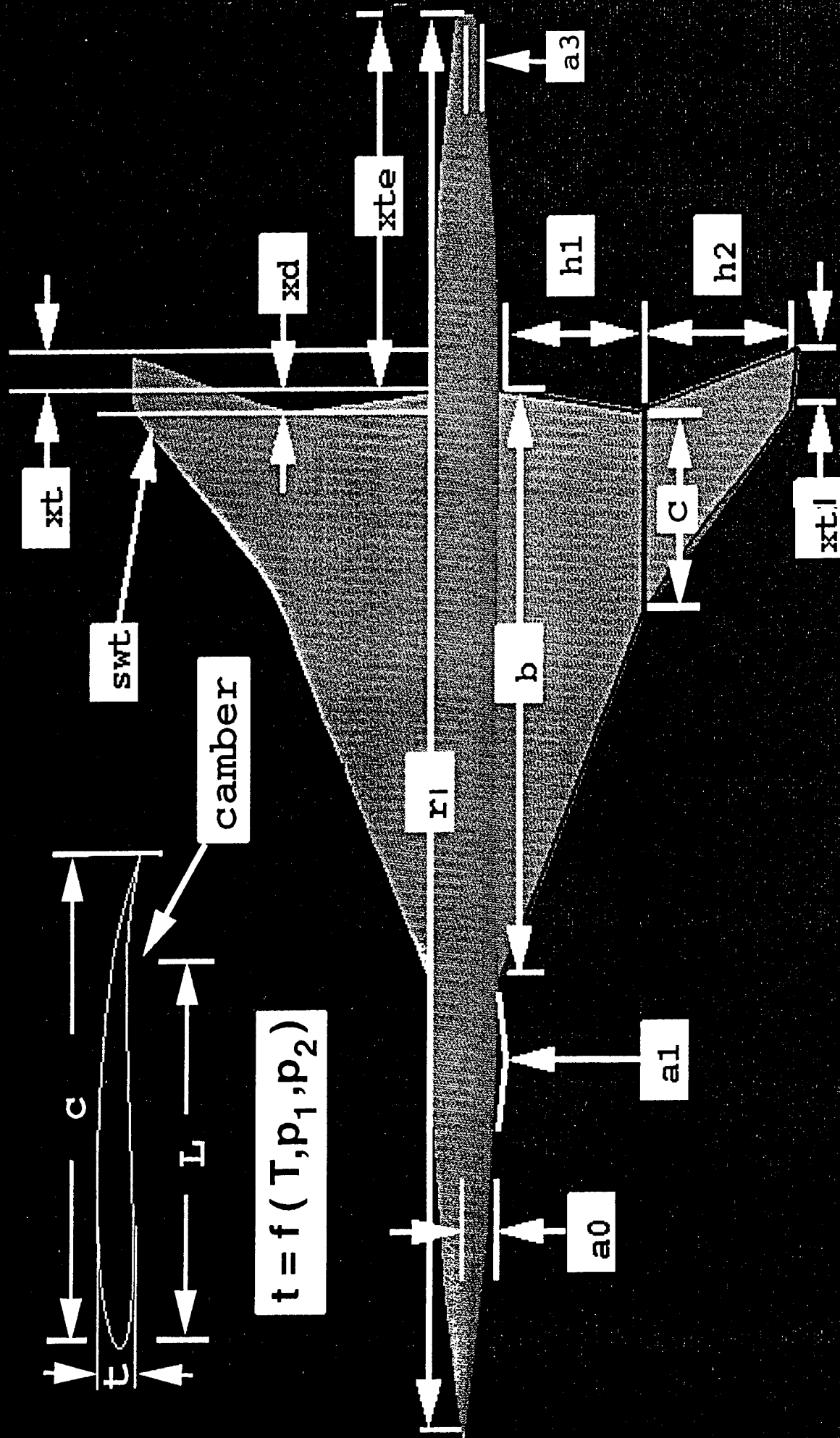


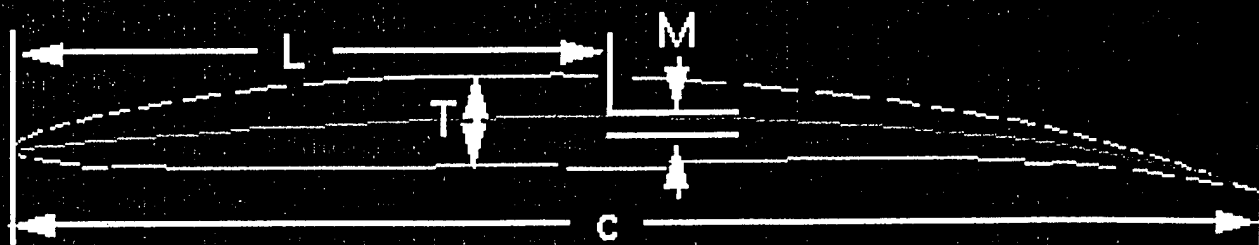
Figure 2: Surface Fitting

AIRPLANE PHYSICAL PARAMETERIZATION



1. Camber curve

2. Thickness distribution



$$x = c \sin(\pi v)$$

$$y_{cam} = \frac{M}{L^2} (2Lx - x^2) \quad x \leq L$$

$$y_{cam} = M \frac{(1 - 2L + 2Lx - x^2)}{(1 - L)^2} \quad x \geq L$$

$$y_t = -\frac{T}{2} (\sin(2\pi v) + P_1 \sin(4\pi v) + P_2 \sin(6\pi v))$$

$$y = y_{cam} + y_t$$

Fig. 4 – Airfoil Section Definition

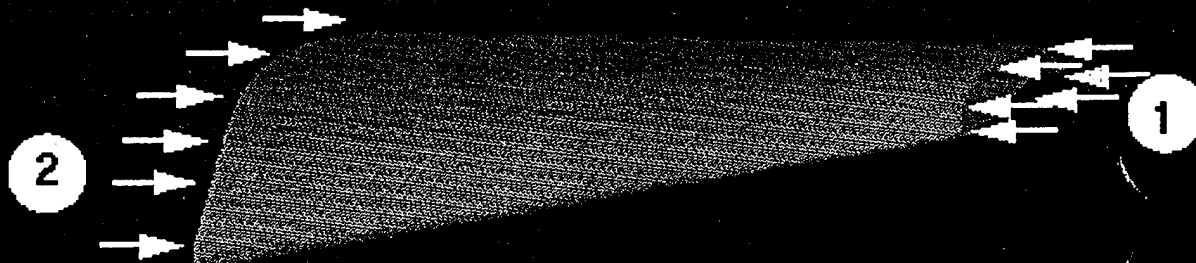
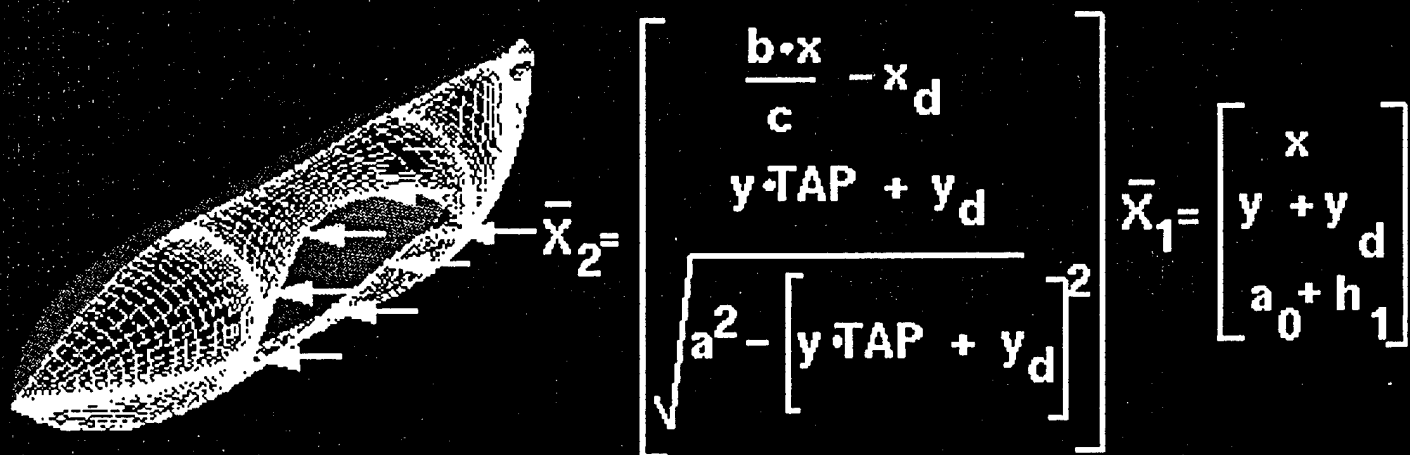


Fig. 5 – Dirichlet Boundary Conditions

$$\frac{\partial \bar{X}_2}{\partial u} = \left[\begin{array}{c} s \frac{\partial y}{\partial v} \sin v \\ -s \frac{\partial x}{\partial v} \sin v \\ \frac{s \frac{\partial y}{\partial v} \sin v \ a \frac{\partial a}{\partial x} - (y_d + y * TAP)(-s \frac{\partial x}{\partial v} \sin v)}{\sqrt{a^2 - (s \frac{\partial x}{\partial v} \sin v)^2}} \end{array} \right]$$

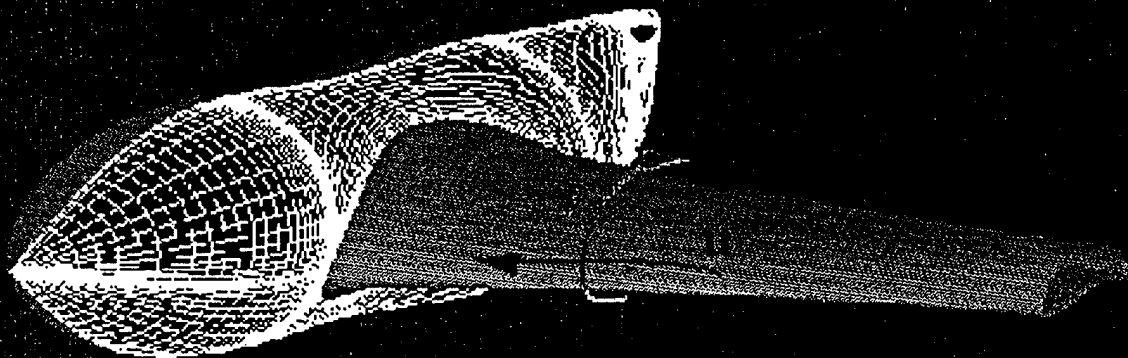


Fig. 6 – Neumann Boundary Conditions

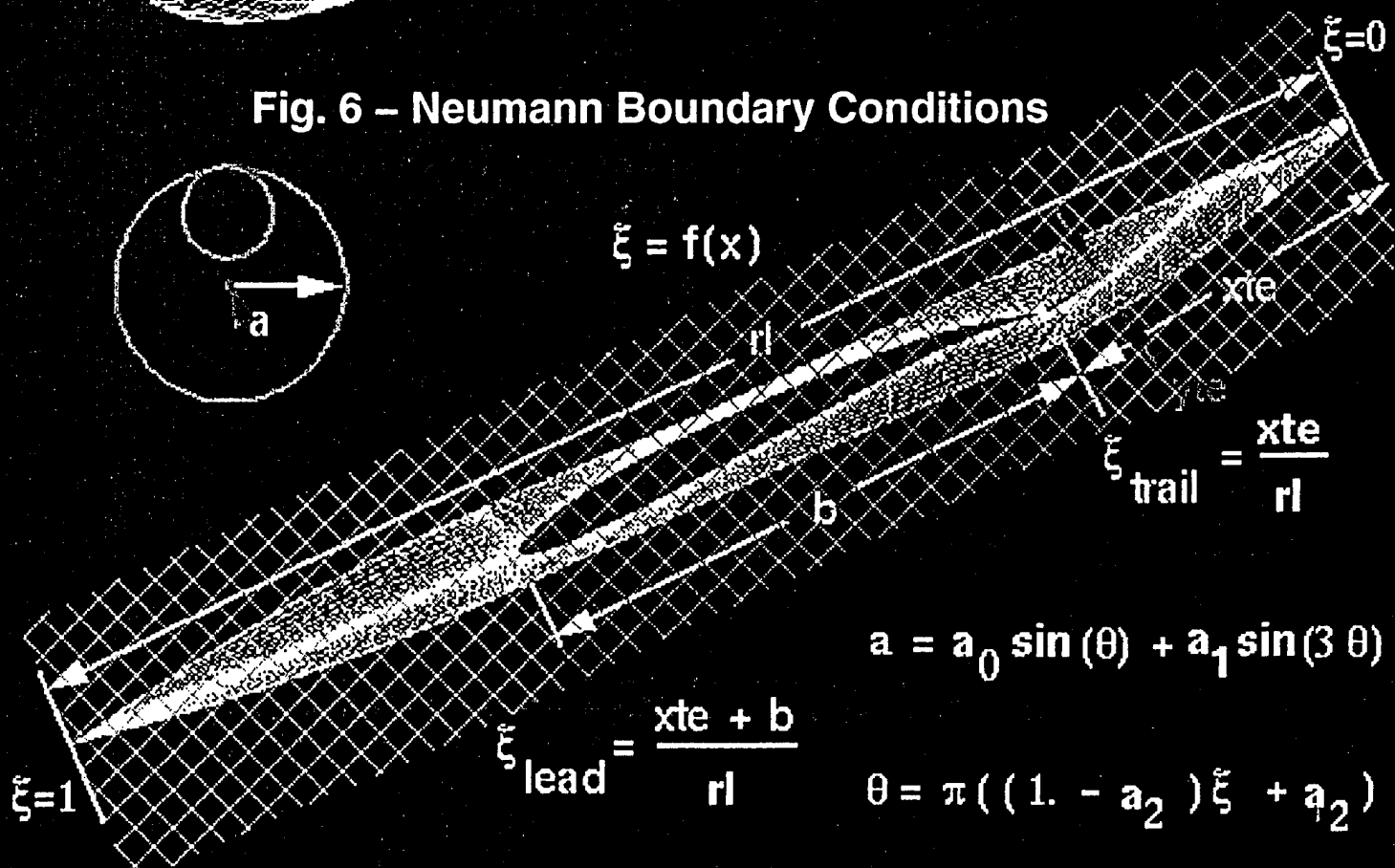


Fig. 7 – Fuselage Definition

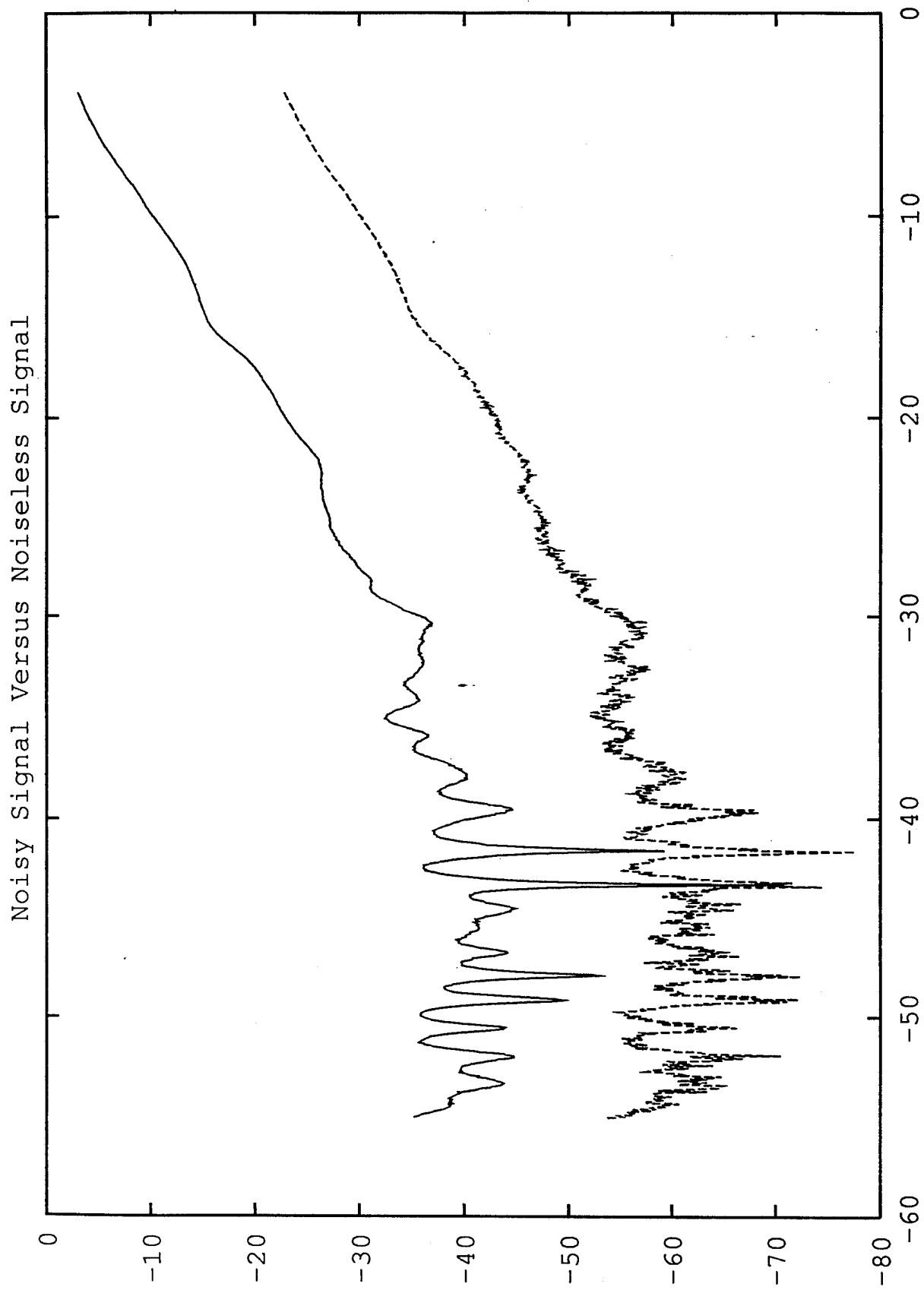


FIGURE 8

Smoothed Signal Versus Noiseless Signal

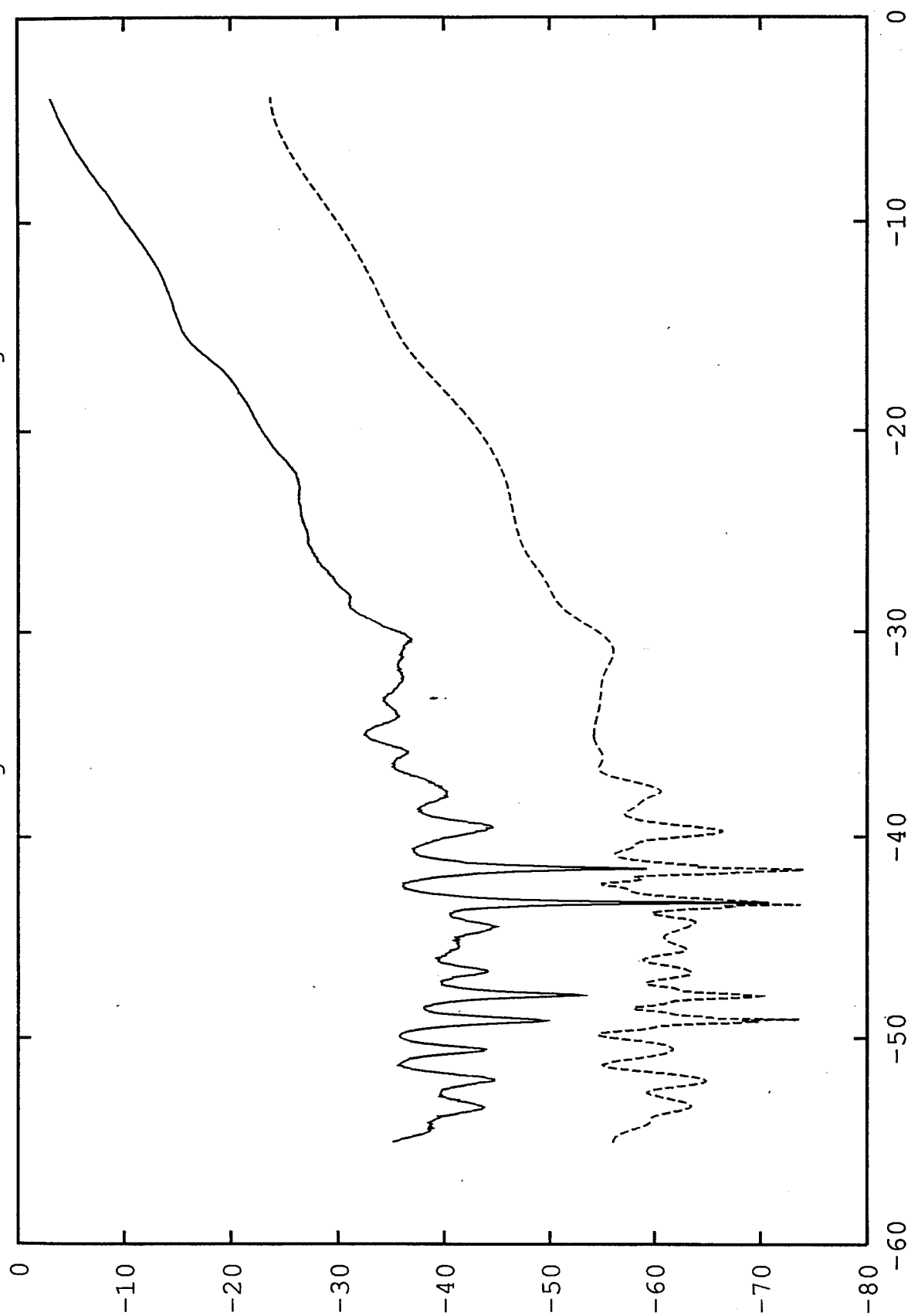


FIGURE 9